



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 4D0M / pdb_00004d0m
Title : Phosphatidylinositol 4-kinase III beta in a complex with Rab11a-GTP-gamma-S and the Rab-binding domain of FIP3
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on : 2014-04-29
Resolution : 6.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

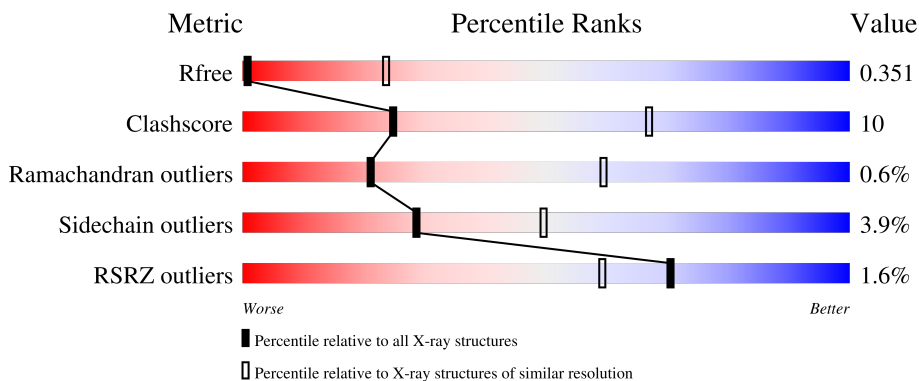
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	 3% 69% 12% 17%
1	C	566	 3% 68% 13% 17%
1	G	566	 0% 69% 13% 17%
1	I	566	 2% 69% 13% 17%







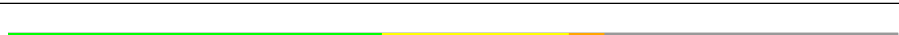
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Mol	Chain	Length	Quality of chain
1	M	566	% 69% 13% 17%
1	O	566	2% 68% 13% 17%
1	Q	566	% 68% 14% 17%
1	S	566	2% 68% 13% 17%
1	W	566	2% 68% 13% 17%
1	Y	566	2% 68% 13% 17%
1	c	566	% 68% 13% 17%
1	g	566	% 68% 14% 17%
2	B	219	60% 18% 21%
2	D	219	% 62% 16% 21%
2	H	219	% 61% 17% 21%
2	J	219	% 63% 16% 21%
2	N	219	62% 16% 21%
2	P	219	61% 17% 21%
2	R	219	3% 61% 17% 21%
2	T	219	% 62% 16% 21%
2	X	219	% 61% 17% 21%
2	Z	219	2% 60% 18% 21%
2	d	219	3% 61% 17% 21%
2	h	219	3% 61% 17% 21%
3	E	48	63% 17% 6% 15%
3	F	48	2% 46% 19% 33%
3	K	48	63% 17% 15%
3	L	48	42% 21% 33%
3	U	48	58% 23% 15%

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Mol	Chain	Length	Quality of chain
3	V	48	
3	a	48	
3	b	48	
3	e	48	
3	f	48	
3	i	48	
3	j	48	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GSP	d	2000	-	-	X	-
6	MG	Z	2001	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 65970 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	470	3788	2430	654	680	24	0	0	0
1	C	470	3788	2430	654	680	24	0	0	0
1	G	470	3788	2430	654	680	24	0	0	0
1	I	470	3788	2430	654	680	24	0	0	0
1	M	470	3788	2430	654	680	24	0	0	0
1	O	470	3788	2430	654	680	24	0	0	0
1	Q	470	3788	2430	654	680	24	0	0	0
1	S	470	3788	2430	654	680	24	0	0	0
1	W	470	3788	2430	654	680	24	0	0	0
1	Y	470	3788	2430	654	680	24	0	0	0
1	c	470	3788	2430	654	680	24	0	0	0
1	g	470	3788	2430	654	680	24	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP Q9UBF8
A	120	SER	-	expression tag	UNP Q9UBF8
A	294	ALA	SER	engineered mutation	UNP Q9UBF8
A	507	ARG	LYS	conflict	UNP Q9UBF8
C	119	GLY	-	expression tag	UNP Q9UBF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	120	SER	-	expression tag	UNP Q9UBF8
C	294	ALA	SER	engineered mutation	UNP Q9UBF8
C	507	ARG	LYS	conflict	UNP Q9UBF8
G	119	GLY	-	expression tag	UNP Q9UBF8
G	120	SER	-	expression tag	UNP Q9UBF8
G	294	ALA	SER	engineered mutation	UNP Q9UBF8
G	507	ARG	LYS	conflict	UNP Q9UBF8
I	119	GLY	-	expression tag	UNP Q9UBF8
I	120	SER	-	expression tag	UNP Q9UBF8
I	294	ALA	SER	engineered mutation	UNP Q9UBF8
I	507	ARG	LYS	conflict	UNP Q9UBF8
M	119	GLY	-	expression tag	UNP Q9UBF8
M	120	SER	-	expression tag	UNP Q9UBF8
M	294	ALA	SER	engineered mutation	UNP Q9UBF8
M	507	ARG	LYS	conflict	UNP Q9UBF8
O	119	GLY	-	expression tag	UNP Q9UBF8
O	120	SER	-	expression tag	UNP Q9UBF8
O	294	ALA	SER	engineered mutation	UNP Q9UBF8
O	507	ARG	LYS	conflict	UNP Q9UBF8
Q	119	GLY	-	expression tag	UNP Q9UBF8
Q	120	SER	-	expression tag	UNP Q9UBF8
Q	294	ALA	SER	engineered mutation	UNP Q9UBF8
Q	507	ARG	LYS	conflict	UNP Q9UBF8
S	119	GLY	-	expression tag	UNP Q9UBF8
S	120	SER	-	expression tag	UNP Q9UBF8
S	294	ALA	SER	engineered mutation	UNP Q9UBF8
S	507	ARG	LYS	conflict	UNP Q9UBF8
W	119	GLY	-	expression tag	UNP Q9UBF8
W	120	SER	-	expression tag	UNP Q9UBF8
W	294	ALA	SER	engineered mutation	UNP Q9UBF8
W	507	ARG	LYS	conflict	UNP Q9UBF8
Y	119	GLY	-	expression tag	UNP Q9UBF8
Y	120	SER	-	expression tag	UNP Q9UBF8
Y	294	ALA	SER	engineered mutation	UNP Q9UBF8
Y	507	ARG	LYS	conflict	UNP Q9UBF8
c	119	GLY	-	expression tag	UNP Q9UBF8
c	120	SER	-	expression tag	UNP Q9UBF8
c	294	ALA	SER	engineered mutation	UNP Q9UBF8
c	507	ARG	LYS	conflict	UNP Q9UBF8
g	119	GLY	-	expression tag	UNP Q9UBF8
g	120	SER	-	expression tag	UNP Q9UBF8
g	294	ALA	SER	engineered mutation	UNP Q9UBF8

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Chain	Residue	Modelled	Actual	Comment	Reference
g	507	ARG	LYS	conflict	UNP Q9UBF8

- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	173	1377	872	238	266	1	0	0	0
2	D	173	1377	872	238	266	1	0	0	0
2	H	173	1377	872	238	266	1	0	0	0
2	J	173	1377	872	238	266	1	0	0	0
2	N	173	1377	872	238	266	1	0	0	0
2	P	173	1377	872	238	266	1	0	0	0
2	R	173	1377	872	238	266	1	0	0	0
2	T	173	1377	872	238	266	1	0	0	0
2	X	173	1377	872	238	266	1	0	0	0
2	Z	173	1377	872	238	266	1	0	0	0
2	d	173	1377	872	238	266	1	0	0	0
2	h	173	1377	872	238	266	1	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62491
B	-1	SER	-	expression tag	UNP P62491
B	0	HIS	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491
D	-2	GLY	-	expression tag	UNP P62491
D	-1	SER	-	expression tag	UNP P62491
D	0	HIS	-	expression tag	UNP P62491
D	70	LEU	GLN	engineered mutation	UNP P62491
H	-2	GLY	-	expression tag	UNP P62491

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	expression tag	UNP P62491
H	0	HIS	-	expression tag	UNP P62491
H	70	LEU	GLN	engineered mutation	UNP P62491
J	-2	GLY	-	expression tag	UNP P62491
J	-1	SER	-	expression tag	UNP P62491
J	0	HIS	-	expression tag	UNP P62491
J	70	LEU	GLN	engineered mutation	UNP P62491
N	-2	GLY	-	expression tag	UNP P62491
N	-1	SER	-	expression tag	UNP P62491
N	0	HIS	-	expression tag	UNP P62491
N	70	LEU	GLN	engineered mutation	UNP P62491
P	-2	GLY	-	expression tag	UNP P62491
P	-1	SER	-	expression tag	UNP P62491
P	0	HIS	-	expression tag	UNP P62491
P	70	LEU	GLN	engineered mutation	UNP P62491
R	-2	GLY	-	expression tag	UNP P62491
R	-1	SER	-	expression tag	UNP P62491
R	0	HIS	-	expression tag	UNP P62491
R	70	LEU	GLN	engineered mutation	UNP P62491
T	-2	GLY	-	expression tag	UNP P62491
T	-1	SER	-	expression tag	UNP P62491
T	0	HIS	-	expression tag	UNP P62491
T	70	LEU	GLN	engineered mutation	UNP P62491
X	-2	GLY	-	expression tag	UNP P62491
X	-1	SER	-	expression tag	UNP P62491
X	0	HIS	-	expression tag	UNP P62491
X	70	LEU	GLN	engineered mutation	UNP P62491
Z	-2	GLY	-	expression tag	UNP P62491
Z	-1	SER	-	expression tag	UNP P62491
Z	0	HIS	-	expression tag	UNP P62491
Z	70	LEU	GLN	engineered mutation	UNP P62491
d	-2	GLY	-	expression tag	UNP P62491
d	-1	SER	-	expression tag	UNP P62491
d	0	HIS	-	expression tag	UNP P62491
d	70	LEU	GLN	engineered mutation	UNP P62491
h	-2	GLY	-	expression tag	UNP P62491
h	-1	SER	-	expression tag	UNP P62491
h	0	HIS	-	expression tag	UNP P62491
h	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	41	314	199	54	60	1	0	0	0
3	F	32	237	153	41	42	1	0	0	0
3	K	41	314	199	54	60	1	0	0	0
3	L	32	237	153	41	42	1	0	0	0
3	U	41	314	199	54	60	1	0	0	0
3	V	32	237	153	41	42	1	0	0	0
3	a	41	314	199	54	60	1	0	0	0
3	b	32	237	153	41	42	1	0	0	0
3	e	41	314	199	54	60	1	0	0	0
3	f	32	237	153	41	42	1	0	0	0
3	i	41	314	199	54	60	1	0	0	0
3	j	32	237	153	41	42	1	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

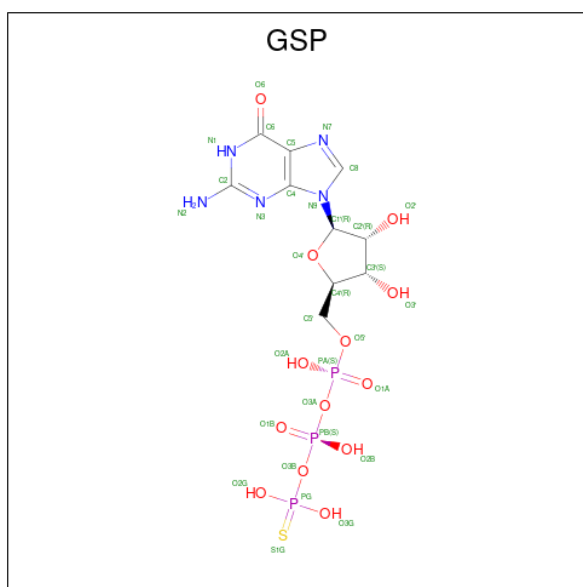
Chain	Residue	Modelled	Actual	Comment	Reference
E	709	GLY	-	expression tag	UNP O75154
E	710	SER	-	expression tag	UNP O75154
E	711	HIS	-	expression tag	UNP O75154
E	712	MET	-	expression tag	UNP O75154
F	709	GLY	-	expression tag	UNP O75154
F	710	SER	-	expression tag	UNP O75154
F	711	HIS	-	expression tag	UNP O75154
F	712	MET	-	expression tag	UNP O75154
K	709	GLY	-	expression tag	UNP O75154
K	710	SER	-	expression tag	UNP O75154
K	711	HIS	-	expression tag	UNP O75154
K	712	MET	-	expression tag	UNP O75154
L	709	GLY	-	expression tag	UNP O75154
L	710	SER	-	expression tag	UNP O75154
L	711	HIS	-	expression tag	UNP O75154
L	712	MET	-	expression tag	UNP O75154

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Chain	Residue	Modelled	Actual	Comment	Reference
U	709	GLY	-	expression tag	UNP O75154
U	710	SER	-	expression tag	UNP O75154
U	711	HIS	-	expression tag	UNP O75154
U	712	MET	-	expression tag	UNP O75154
V	709	GLY	-	expression tag	UNP O75154
V	710	SER	-	expression tag	UNP O75154
V	711	HIS	-	expression tag	UNP O75154
V	712	MET	-	expression tag	UNP O75154
a	709	GLY	-	expression tag	UNP O75154
a	710	SER	-	expression tag	UNP O75154
a	711	HIS	-	expression tag	UNP O75154
a	712	MET	-	expression tag	UNP O75154
b	709	GLY	-	expression tag	UNP O75154
b	710	SER	-	expression tag	UNP O75154
b	711	HIS	-	expression tag	UNP O75154
b	712	MET	-	expression tag	UNP O75154
e	709	GLY	-	expression tag	UNP O75154
e	710	SER	-	expression tag	UNP O75154
e	711	HIS	-	expression tag	UNP O75154
e	712	MET	-	expression tag	UNP O75154
f	709	GLY	-	expression tag	UNP O75154
f	710	SER	-	expression tag	UNP O75154
f	711	HIS	-	expression tag	UNP O75154
f	712	MET	-	expression tag	UNP O75154
i	709	GLY	-	expression tag	UNP O75154
i	710	SER	-	expression tag	UNP O75154
i	711	HIS	-	expression tag	UNP O75154
i	712	MET	-	expression tag	UNP O75154
j	709	GLY	-	expression tag	UNP O75154
j	710	SER	-	expression tag	UNP O75154
j	711	HIS	-	expression tag	UNP O75154
j	712	MET	-	expression tag	UNP O75154

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (CCD ID: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
5	B	1	Total 32	10	5	13	3	1	0	0
5	D	1	Total 32	10	5	13	3	1	0	0
5	H	1	Total 32	10	5	13	3	1	0	0
5	J	1	Total 32	10	5	13	3	1	0	0
5	N	1	Total 32	10	5	13	3	1	0	0
5	P	1	Total 32	10	5	13	3	1	0	0
5	R	1	Total 32	10	5	13	3	1	0	0
5	T	1	Total 32	10	5	13	3	1	0	0
5	X	1	Total 32	10	5	13	3	1	0	0
5	Z	1	Total 32	10	5	13	3	1	0	0
5	d	1	Total 32	10	5	13	3	1	0	0
5	h	1	Total 32	10	5	13	3	1	0	0

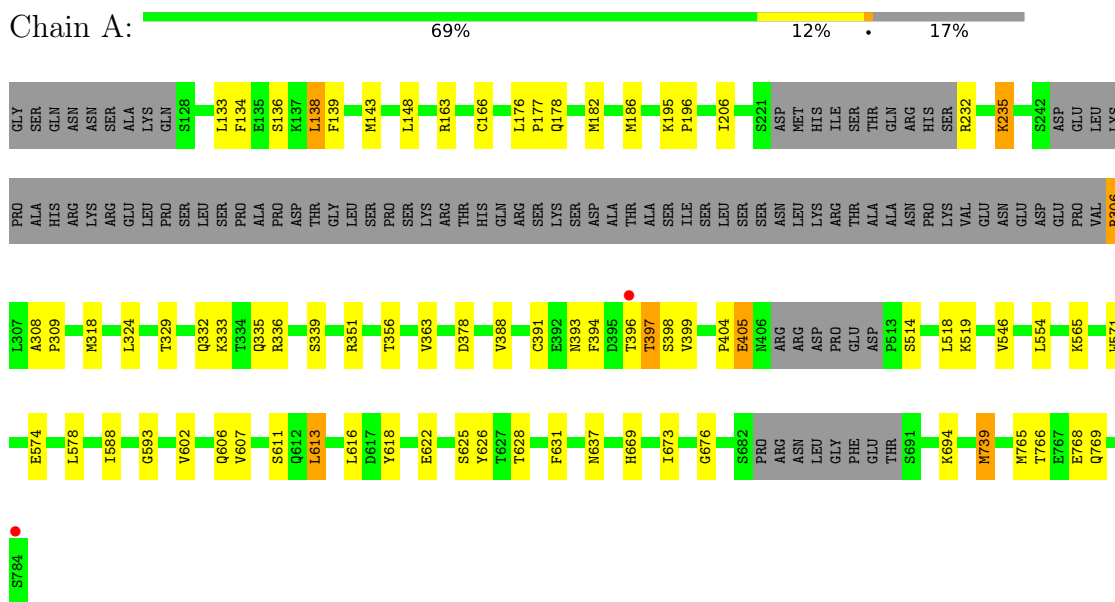
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	H	1	Total Mg 1 1	0	0
6	J	1	Total Mg 1 1	0	0
6	N	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0
6	R	1	Total Mg 1 1	0	0
6	T	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	Z	1	Total Mg 1 1	0	0
6	d	1	Total Mg 1 1	0	0
6	h	1	Total Mg 1 1	0	0

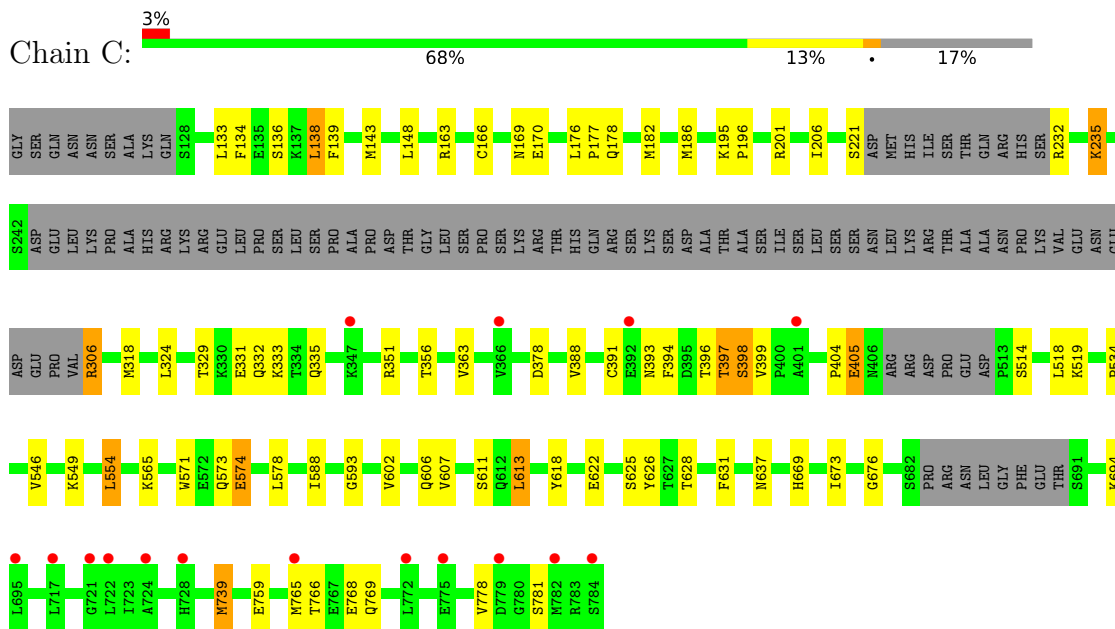
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

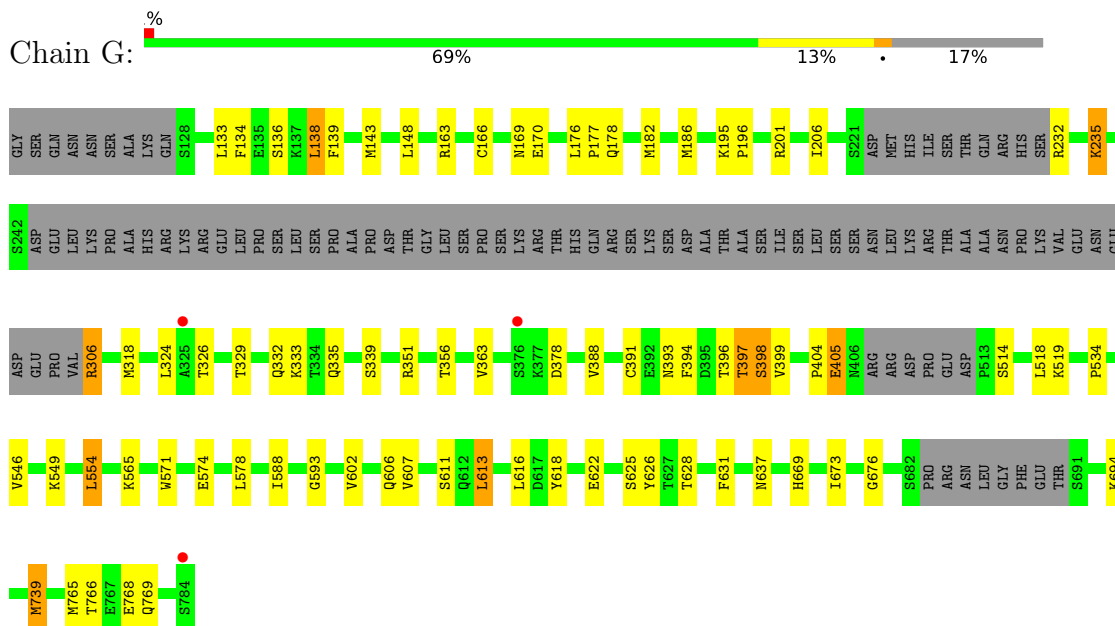
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



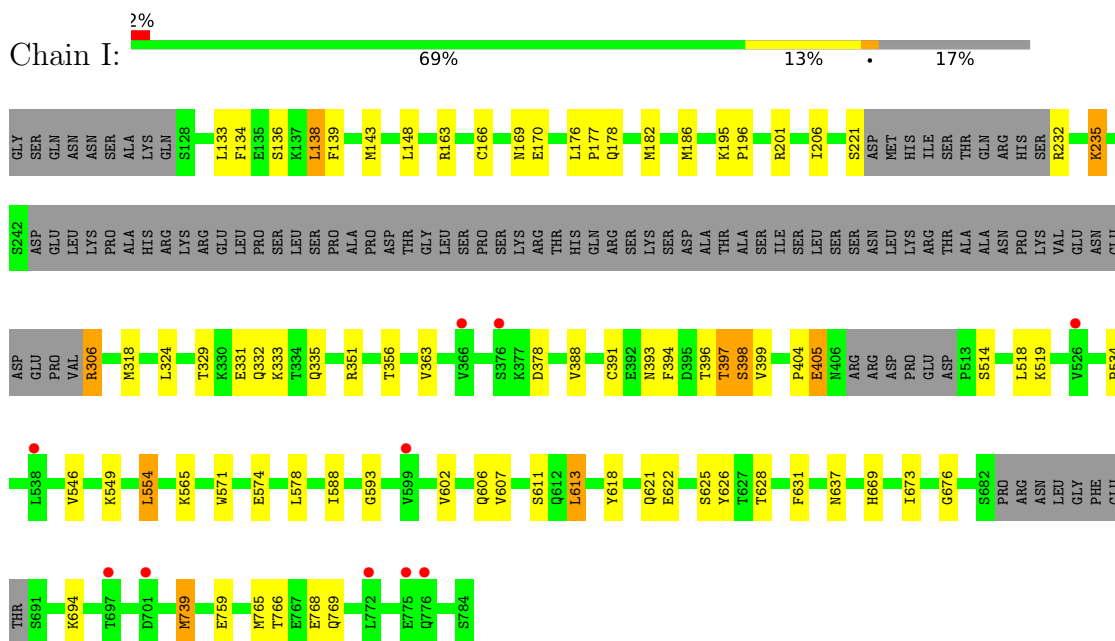
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



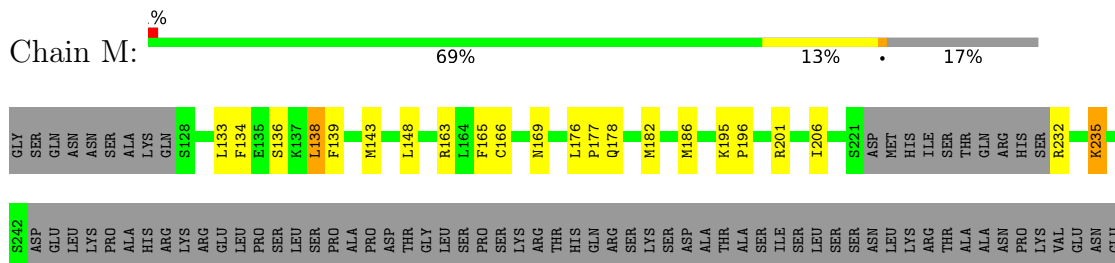
- Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

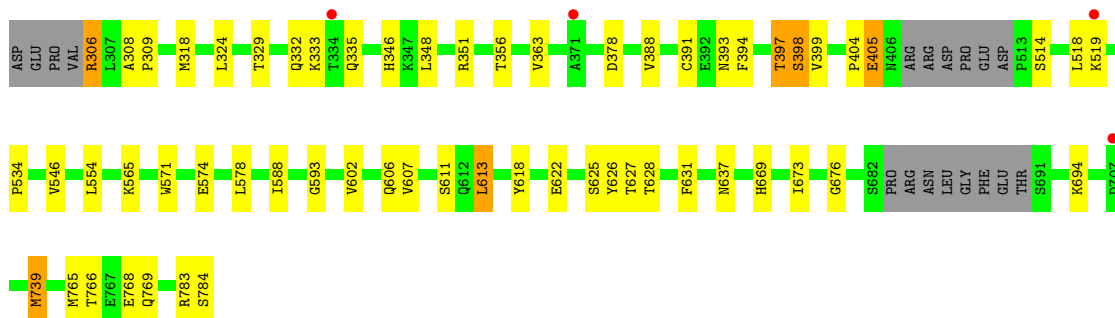


- Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

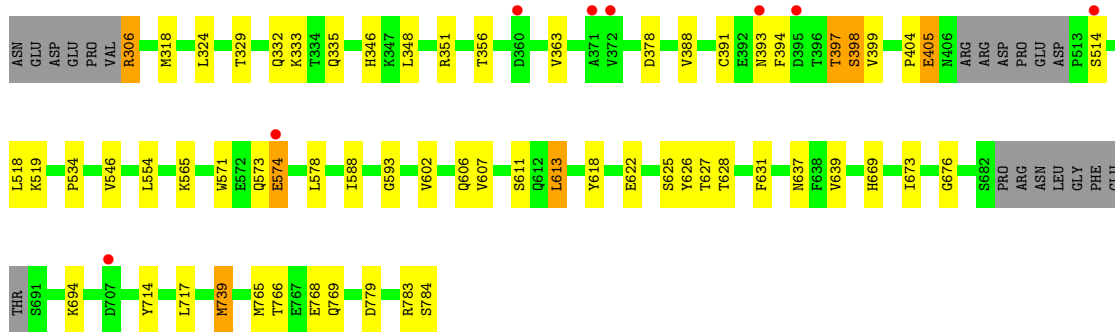
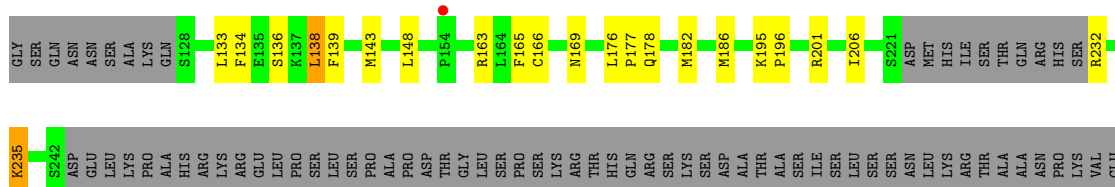


- Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

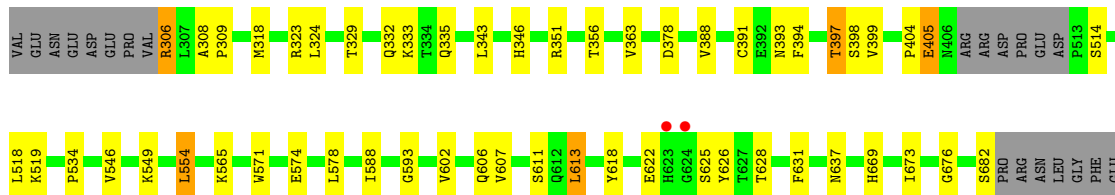
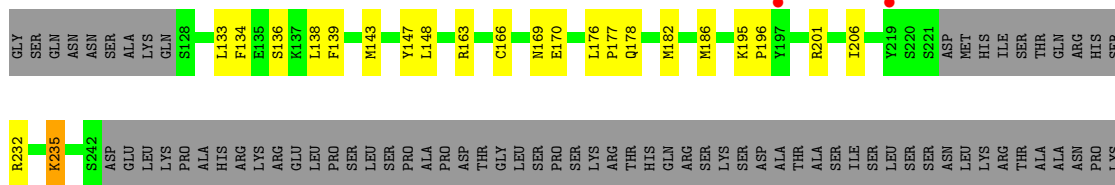


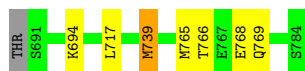


● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

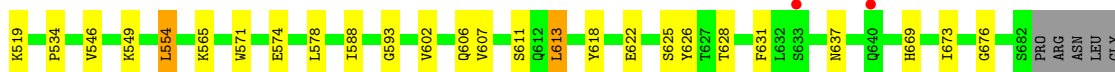
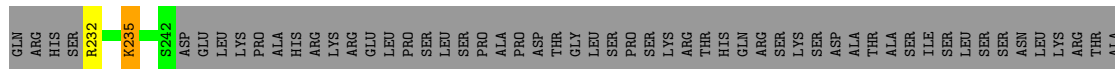


● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

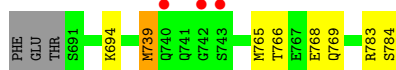
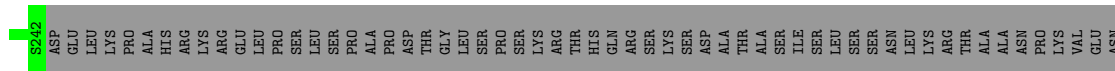




● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

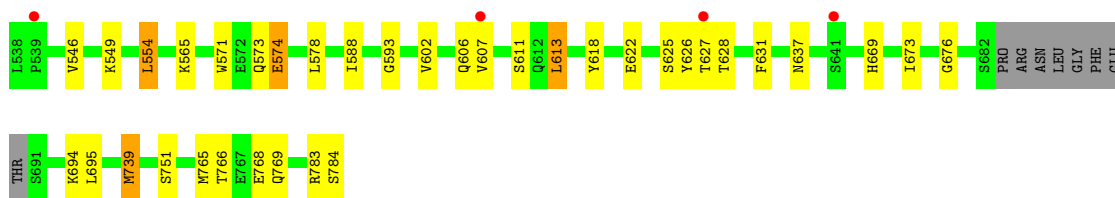


● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

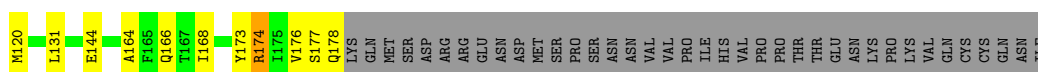


● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

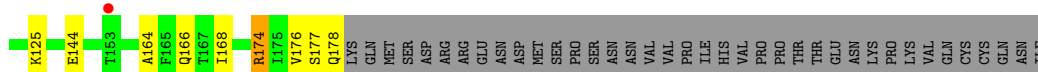




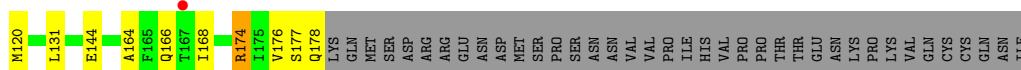
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



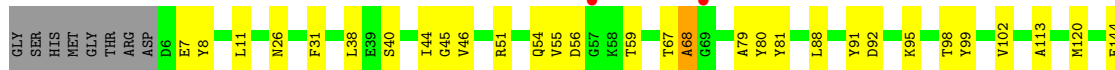
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



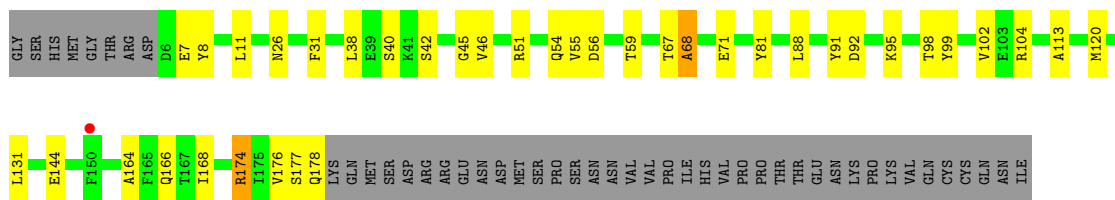
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



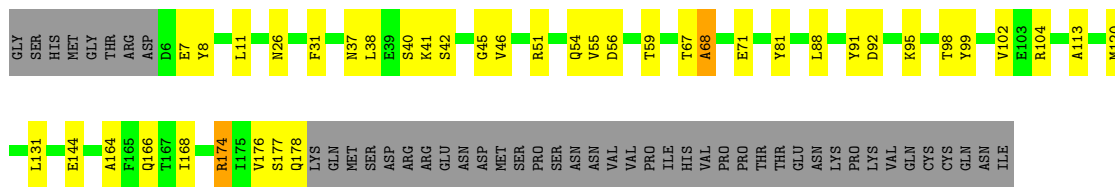
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



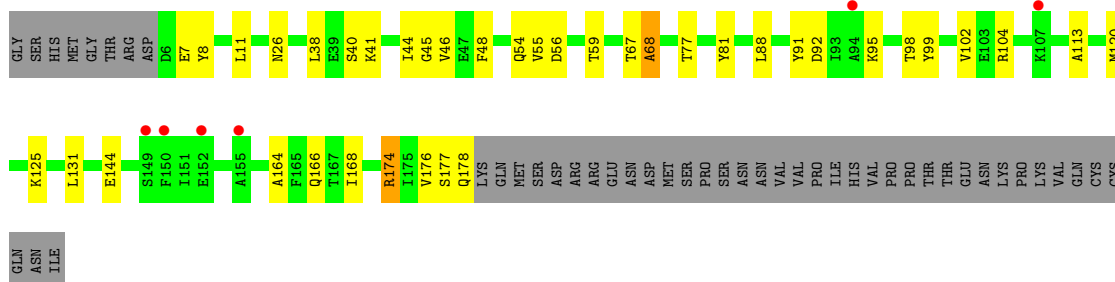
● Molecule 2: RAS-RELATED PROTEIN RAB-11A



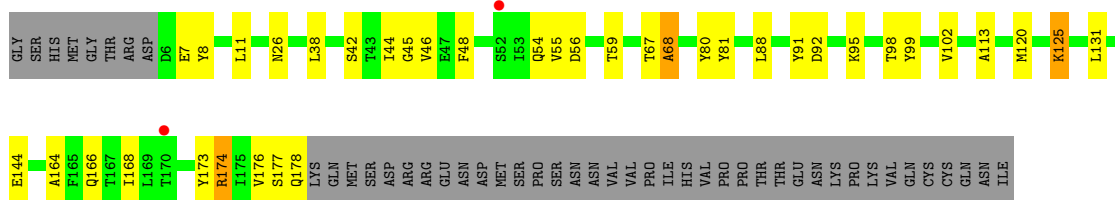
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

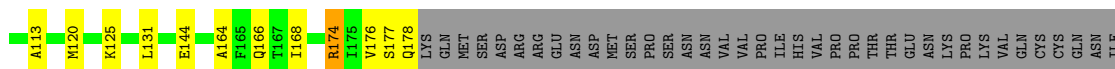


• Molecule 2: RAS-RELATED PROTEIN RAB-11A

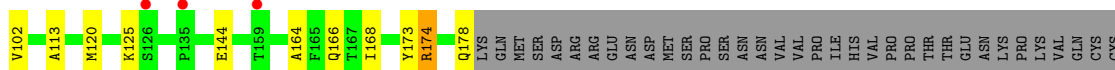
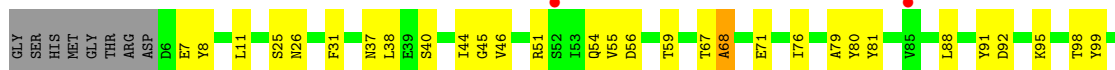


• Molecule 2: RAS-RELATED PROTEIN RAB-11A



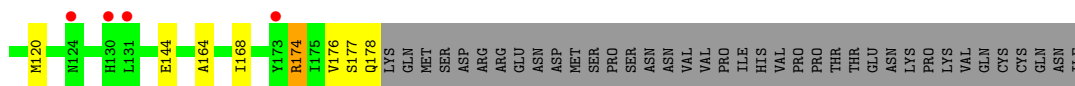


- Molecule 2: RAS-RELATED PROTEIN RAB-11A

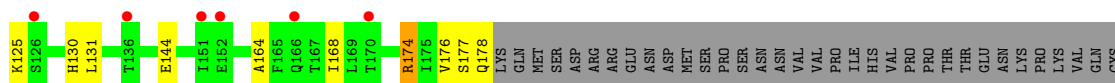
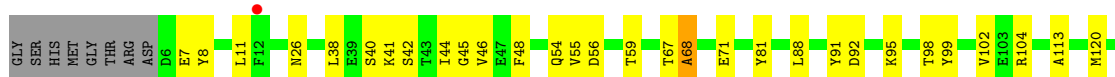


GLN
ASN
ILE

- Molecule 2: RAS-RELATED PROTEIN RAB-11A



- Molecule 2: RAS-RELATED PROTEIN RAB-11A



CYS
GLN
ASN
ILE

- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

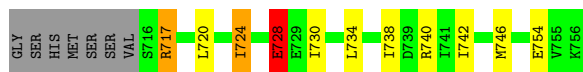


- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

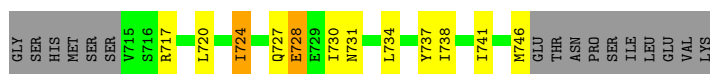




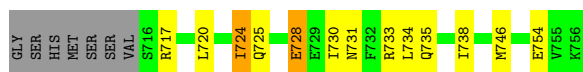
● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

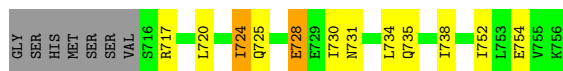


● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

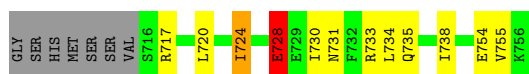




- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



- Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	199.50Å 134.47Å 294.33Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	294.32 – 6.00 294.32 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (294.32-6.00) 92.8 (294.32-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 6.15Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.253 , 0.359 0.252 , 0.351	Depositor DCC
R_{free} test set	2048 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	248.6	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 945.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.389 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 093, GSP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/3866	0.95	6/5219 (0.1%)
1	C	0.73	0/3866	0.94	6/5219 (0.1%)
1	G	0.74	0/3866	0.95	6/5219 (0.1%)
1	I	0.72	0/3866	0.93	5/5219 (0.1%)
1	M	0.74	0/3866	0.95	6/5219 (0.1%)
1	O	0.75	0/3866	0.95	6/5219 (0.1%)
1	Q	0.73	0/3866	0.95	6/5219 (0.1%)
1	S	0.73	0/3866	0.94	6/5219 (0.1%)
1	W	0.75	0/3866	0.94	6/5219 (0.1%)
1	Y	0.74	0/3866	0.94	2/5219 (0.0%)
1	c	0.77	0/3866	0.95	4/5219 (0.1%)
1	g	0.75	0/3866	0.94	6/5219 (0.1%)
2	B	0.82	0/1399	0.98	1/1892 (0.1%)
2	D	0.81	0/1399	0.96	0/1892
2	H	0.80	0/1399	0.97	0/1892
2	J	0.82	0/1399	0.97	0/1892
2	N	0.77	0/1399	0.94	0/1892
2	P	0.77	0/1399	0.94	0/1892
2	R	0.76	0/1399	0.94	1/1892 (0.1%)
2	T	0.75	0/1399	0.94	0/1892
2	X	0.76	0/1399	0.94	0/1892
2	Z	0.77	0/1399	0.93	0/1892
2	d	0.77	0/1399	0.94	1/1892 (0.1%)
2	h	0.78	0/1399	0.93	0/1892
3	E	1.23	2/316 (0.6%)	1.25	1/429 (0.2%)
3	F	1.18	1/238 (0.4%)	1.23	0/323
3	K	1.24	2/316 (0.6%)	1.25	1/429 (0.2%)
3	L	1.20	2/238 (0.8%)	1.24	0/323
3	U	1.11	1/316 (0.3%)	1.13	0/429
3	V	1.26	0/238	1.21	1/323 (0.3%)
3	a	1.25	2/316 (0.6%)	1.24	1/429 (0.2%)
3	b	1.22	0/238	1.21	0/323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	1.15	1/316 (0.3%)	1.15	0/429
3	f	1.24	0/238	1.22	1/323 (0.3%)
3	i	1.16	1/316 (0.3%)	1.15	1/429 (0.2%)
3	j	1.27	0/238	1.19	1/323 (0.3%)
All	All	0.78	12/66504 (0.0%)	0.96	75/89844 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
1	S	0	1
1	W	0	1
1	Y	0	1
1	c	0	1
1	g	0	1
All	All	0	12

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	717	ARG	CD-NE	6.71	1.55	1.46
3	E	717	ARG	CD-NE	6.36	1.55	1.46
3	K	724	ILE	C-O	6.33	1.31	1.24
3	K	717	ARG	CD-NE	6.29	1.55	1.46
3	E	724	ILE	C-O	6.17	1.31	1.24

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	676	GLY	N-CA-C	-8.07	102.21	112.54
1	W	574	GLU	N-CA-C	-8.00	100.28	110.19
1	O	574	GLU	N-CA-C	-7.71	100.63	110.19
1	g	574	GLU	N-CA-C	-7.53	100.85	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	574	GLU	N-CA-C	-7.52	100.86	110.19

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	398	SER	Peptide
1	G	398	SER	Peptide
1	I	398	SER	Peptide
1	M	398	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3788	0	3838	57	8
1	C	3788	0	3839	85	2
1	G	3788	0	3839	54	10
1	I	3788	0	3839	83	2
1	M	3788	0	3839	58	12
1	O	3788	0	3839	59	17
1	Q	3788	0	3839	65	4
1	S	3788	0	3839	67	12
1	W	3788	0	3838	59	4
1	Y	3788	0	3839	60	12
1	c	3788	0	3839	59	7
1	g	3788	0	3839	62	13
2	B	1377	0	1370	47	9
2	D	1377	0	1370	37	4
2	H	1377	0	1370	38	3
2	J	1377	0	1370	36	4
2	N	1377	0	1370	29	0
2	P	1377	0	1371	32	0
2	R	1377	0	1370	32	0
2	T	1377	0	1370	31	0
2	X	1377	0	1370	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	1377	0	1371	40	0
2	d	1377	0	1370	33	0
2	h	1377	0	1370	39	1
3	E	314	0	298	62	0
3	F	237	0	222	29	0
3	K	314	0	298	53	0
3	L	237	0	222	35	0
3	U	314	0	298	23	0
3	V	237	0	222	47	0
3	a	314	0	298	45	0
3	b	237	0	222	33	0
3	e	314	0	298	30	0
3	f	237	0	222	49	0
3	i	314	0	298	33	0
3	j	237	0	222	59	0
4	A	24	0	16	0	0
4	C	24	0	16	0	0
4	G	24	0	16	0	0
4	I	24	0	16	0	0
4	M	24	0	16	0	0
4	O	24	0	16	0	0
4	Q	24	0	16	0	0
4	S	24	0	16	0	0
4	W	24	0	16	0	0
4	Y	24	0	16	0	0
4	c	24	0	16	0	0
4	g	24	0	16	0	0
5	B	32	0	12	6	0
5	D	32	0	12	6	0
5	H	32	0	12	4	0
5	J	32	0	12	4	0
5	N	32	0	12	6	0
5	P	32	0	12	7	0
5	R	32	0	12	6	0
5	T	32	0	12	6	0
5	X	32	0	12	6	0
5	Z	32	0	12	6	0
5	d	32	0	12	11	0
5	h	32	0	12	7	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0
6	T	1	0	0	0	0
6	X	1	0	0	0	0
6	Z	1	0	0	2	0
6	d	1	0	0	0	0
6	h	1	0	0	0	0
All	All	65970	0	65964	1287	62

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1287 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:44:ILE:HD11	3:K:734:LEU:CD2	1.30	1.59
2:J:44:ILE:CD1	3:K:734:LEU:HD22	1.30	1.59
2:D:44:ILE:HD11	3:E:734:LEU:CD2	1.41	1.50
1:C:138:LEU:HG	1:S:769:GLN:CG	1.41	1.48
2:D:44:ILE:CD1	3:E:734:LEU:HD22	1.44	1.47

The worst 5 of 62 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:174:ARG:NH2	1:M:166:CYS:O[2_545]	0.72	1.48
2:D:174:ARG:NH2	1:O:166:CYS:O[2_556]	0.76	1.44
2:B:174:ARG:NH2	1:g:166:CYS:O[2_656]	0.78	1.42
1:I:396:THR:OG1	1:M:627:THR:OG1[2_545]	0.85	1.35
1:C:396:THR:OG1	1:O:627:THR:OG1[2_556]	1.08	1.12

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/566 (81%)	442 (96%)	16 (4%)	2 (0%)	30	67
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	18	56
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	18	56
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	18	56
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	30	67
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	18	56
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	30	67
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	30	67
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	21	59
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	10	44
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	10	44
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
3	E	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	F	30/48 (62%)	30 (100%)	0	0	100	100
3	K	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	L	30/48 (62%)	30 (100%)	0	0	100	100
3	U	39/48 (81%)	38 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	30/48 (62%)	30 (100%)	0	0	100	100
3	a	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	b	30/48 (62%)	30 (100%)	0	0	100	100
3	e	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	f	30/48 (62%)	30 (100%)	0	0	100	100
3	i	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	j	30/48 (62%)	30 (100%)	0	0	100	100
All	All	7986/9996 (80%)	7645 (96%)	295 (4%)	46 (1%)	21	59

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
2	B	68	ALA
1	C	405	GLU
2	D	68	ALA
1	G	405	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	C	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	G	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	I	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	M	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	O	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	Q	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	S	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	W	422/508 (83%)	406 (96%)	16 (4%)	29	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	c	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	g	422/508 (83%)	406 (96%)	16 (4%)	29	50
2	B	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	D	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	H	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	J	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	N	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	P	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	R	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	T	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	X	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	Z	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	d	147/191 (77%)	141 (96%)	6 (4%)	27	48
2	h	147/191 (77%)	141 (96%)	6 (4%)	27	48
3	E	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	F	21/45 (47%)	21 (100%)	0	100	100
3	K	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	L	21/45 (47%)	21 (100%)	0	100	100
3	U	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	V	21/45 (47%)	20 (95%)	1 (5%)	23	44
3	a	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	b	21/45 (47%)	21 (100%)	0	100	100
3	e	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	f	21/45 (47%)	20 (95%)	1 (5%)	23	44
3	i	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	j	21/45 (47%)	20 (95%)	1 (5%)	23	44
All	All	7140/8928 (80%)	6861 (96%)	279 (4%)	28	49

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	728	GLU

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Mol	Chain	Res	Type
1	c	378	ASP
1	g	318	MET
1	M	318	MET
1	M	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	393	ASN
3	e	731	ASN
1	S	162	ASN
1	c	776	GLN
1	g	621	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	093	S	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	14 (42%)
4	093	c	2002	-	25,25,25	3.35	9 (36%)	33,36,36	5.43	15 (45%)
5	GSP	T	2000	6	33,34,34	1.26	3 (9%)	47,54,54	1.99	10 (21%)
4	093	Y	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.43	14 (42%)
5	GSP	R	2000	6	33,34,34	1.44	6 (18%)	47,54,54	1.95	9 (19%)
5	GSP	J	2000	6	33,34,34	1.48	6 (18%)	47,54,54	1.97	11 (23%)
5	GSP	H	2000	6	33,34,34	1.37	4 (12%)	47,54,54	2.06	10 (21%)
5	GSP	X	2000	6	33,34,34	1.42	6 (18%)	47,54,54	2.03	13 (27%)
4	093	C	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.44	14 (42%)
5	GSP	P	2000	6	33,34,34	1.38	6 (18%)	47,54,54	1.95	13 (27%)
4	093	O	2002	-	25,25,25	3.35	9 (36%)	33,36,36	5.43	15 (45%)
4	093	W	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.45	15 (45%)
4	093	M	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	15 (45%)
5	GSP	D	2000	6	33,34,34	1.44	6 (18%)	47,54,54	2.01	10 (21%)
4	093	A	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.45	14 (42%)
5	GSP	B	2000	6	33,34,34	1.44	5 (15%)	47,54,54	2.01	9 (19%)
5	GSP	Z	2000	6	33,34,34	1.40	6 (18%)	47,54,54	1.87	12 (25%)
4	093	Q	2002	-	25,25,25	3.35	9 (36%)	33,36,36	5.43	14 (42%)
5	GSP	d	2000	6	33,34,34	1.42	6 (18%)	47,54,54	1.93	9 (19%)
4	093	g	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	13 (39%)
5	GSP	h	2000	6	33,34,34	1.44	5 (15%)	47,54,54	2.10	12 (25%)
5	GSP	N	2000	6	33,34,34	1.33	7 (21%)	47,54,54	1.91	11 (23%)
4	093	I	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	14 (42%)
4	093	G	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.44	14 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	093	S	2002	-	-	8/19/19/19	0/2/2/2
4	093	c	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	T	2000	6	-	3/21/38/38	0/3/3/3
4	093	Y	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	R	2000	6	-	3/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	J	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	H	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	X	2000	6	-	3/21/38/38	0/3/3/3
4	093	C	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	P	2000	6	-	3/21/38/38	0/3/3/3
4	093	O	2002	-	-	8/19/19/19	0/2/2/2
4	093	W	2002	-	-	8/19/19/19	0/2/2/2
4	093	M	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	D	2000	6	-	3/21/38/38	0/3/3/3
4	093	A	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	B	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	Z	2000	6	-	3/21/38/38	0/3/3/3
4	093	Q	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	d	2000	6	-	3/21/38/38	0/3/3/3
4	093	g	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	h	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	N	2000	6	-	3/21/38/38	0/3/3/3
4	093	I	2002	-	-	8/19/19/19	0/2/2/2
4	093	G	2002	-	-	8/19/19/19	0/2/2/2

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2002	093	CAQ-SAP	-8.79	1.59	1.73
4	Q	2002	093	CAQ-SAP	-8.78	1.59	1.73
4	S	2002	093	CAQ-SAP	-8.76	1.59	1.73
4	A	2002	093	CAQ-SAP	-8.75	1.59	1.73
4	W	2002	093	CAQ-SAP	-8.74	1.59	1.73

The worst 5 of 300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	OAO-SAN-OAM	-20.60	94.51	119.52
4	g	2002	093	OAO-SAN-OAM	-20.57	94.53	119.52
4	Q	2002	093	OAO-SAN-OAM	-20.56	94.55	119.52
4	G	2002	093	OAO-SAN-OAM	-20.55	94.56	119.52
4	C	2002	093	OAO-SAN-OAM	-20.55	94.56	119.52

There are no chirality outliers.

5 of 132 torsion outliers are listed below:

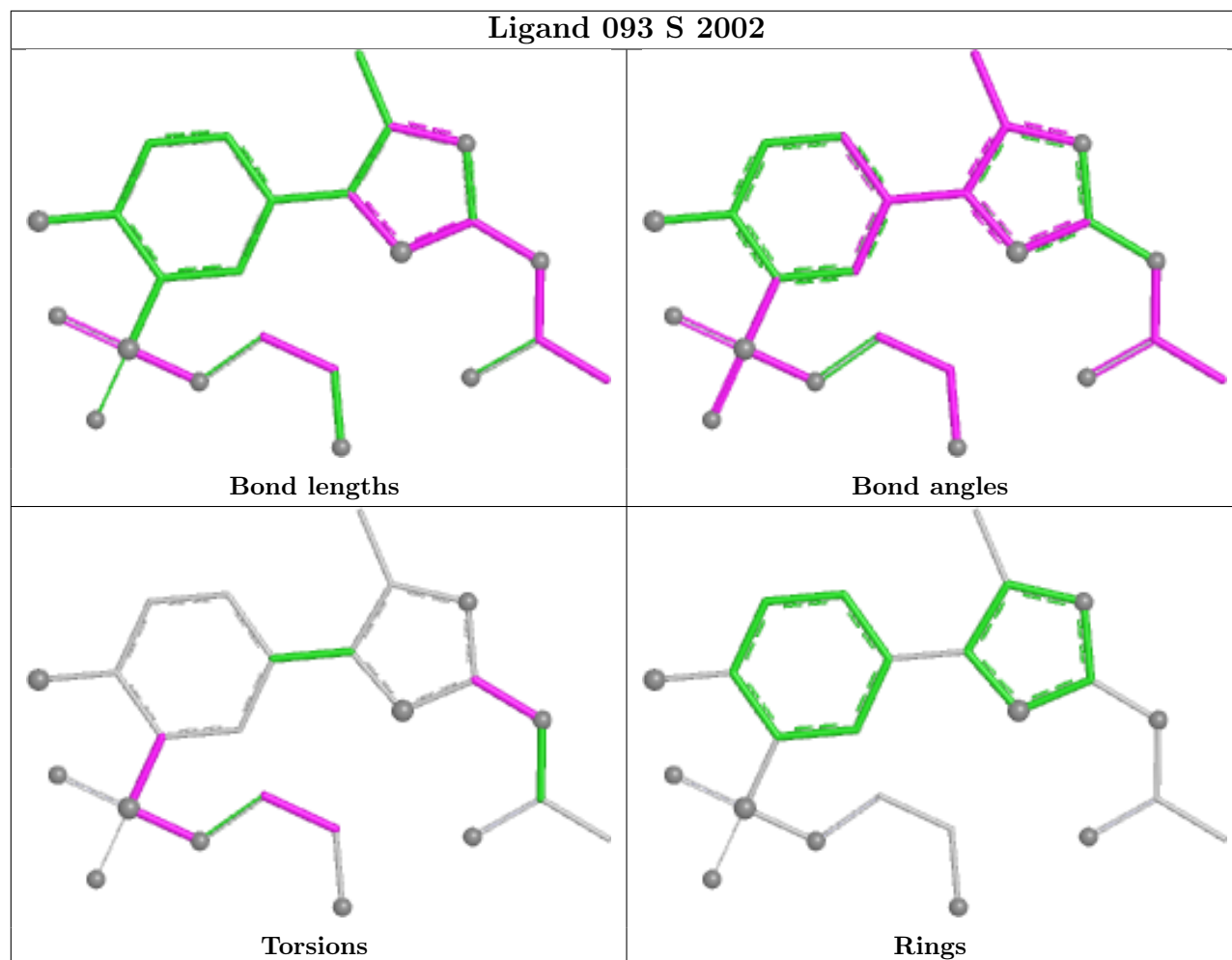
Mol	Chain	Res	Type	Atoms
4	A	2002	093	NAK-CAQ-NAR-CAS
4	A	2002	093	SAP-CAQ-NAR-CAS
4	C	2002	093	NAK-CAQ-NAR-CAS
4	C	2002	093	SAP-CAQ-NAR-CAS
4	G	2002	093	NAK-CAQ-NAR-CAS

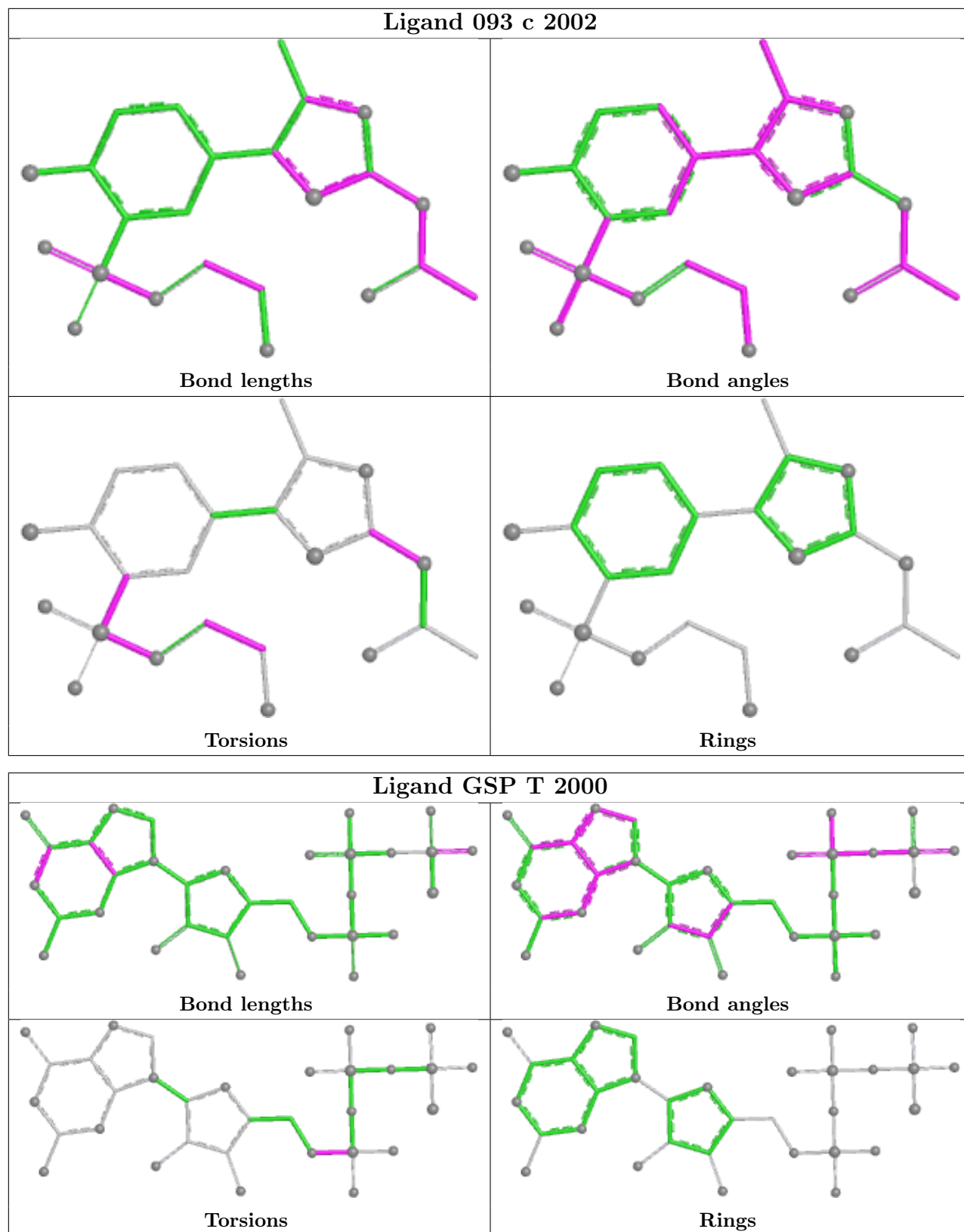
There are no ring outliers.

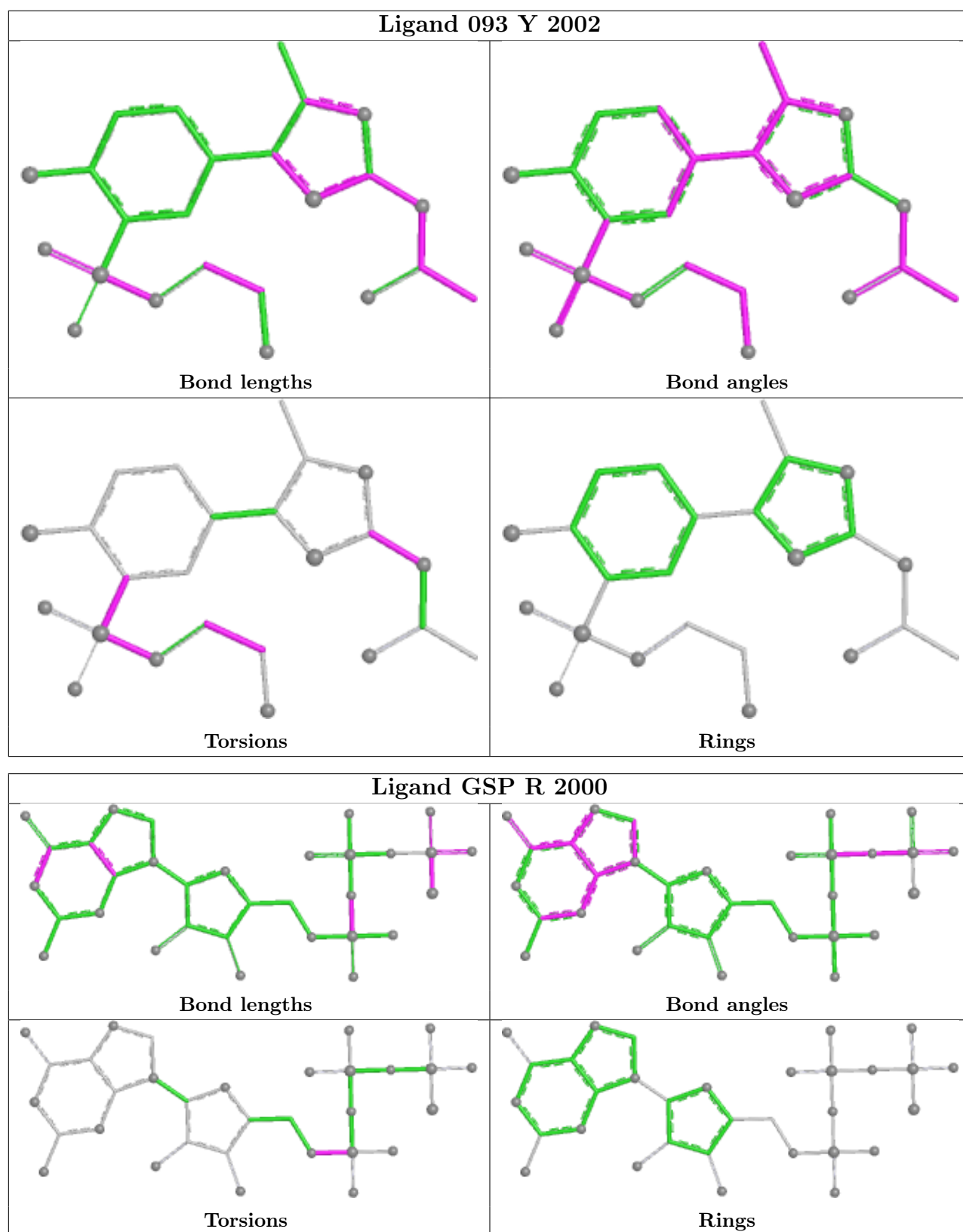
12 monomers are involved in 75 short contacts:

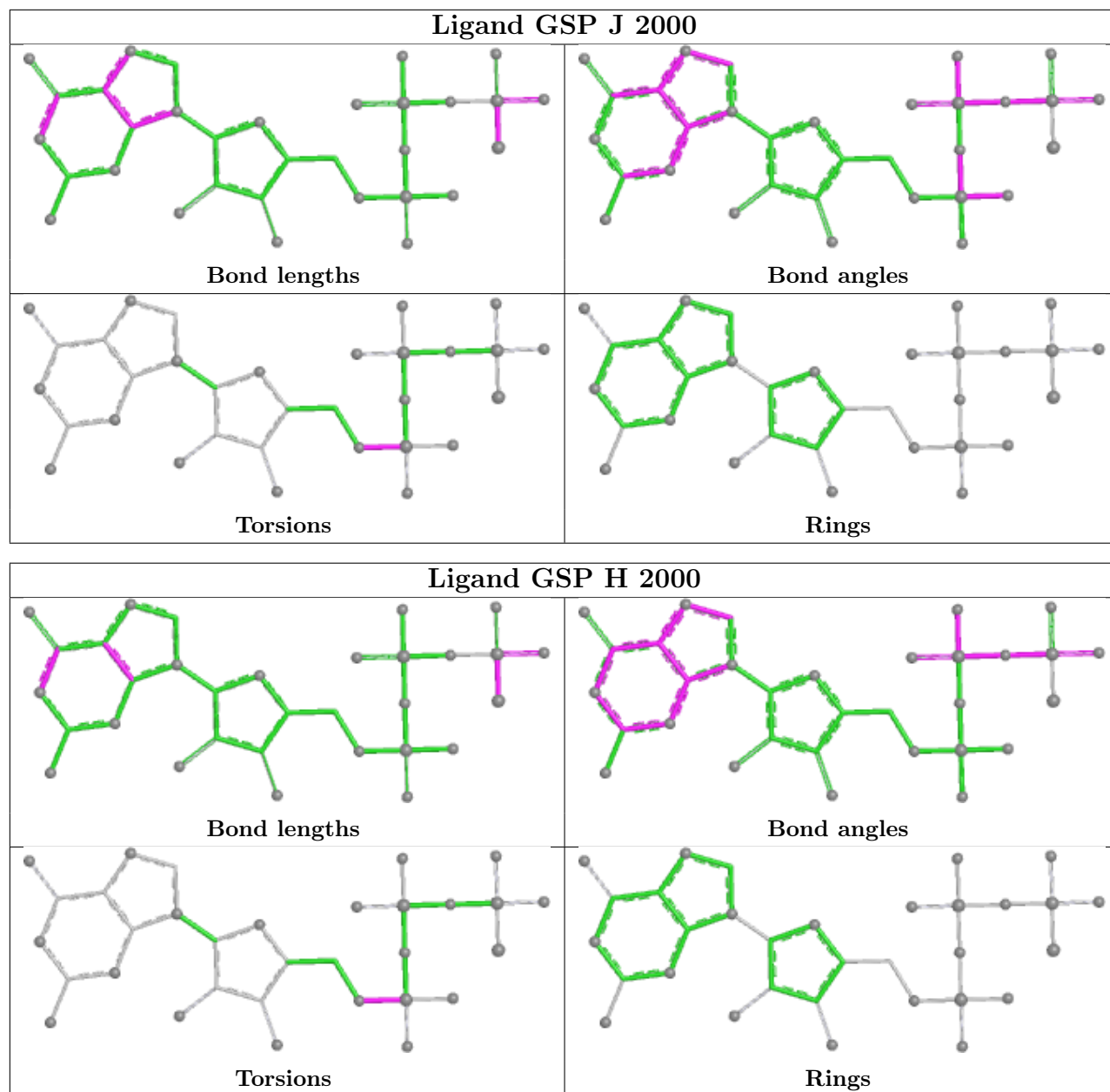
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2000	GSP	6	0
5	R	2000	GSP	6	0
5	J	2000	GSP	4	0
5	H	2000	GSP	4	0
5	X	2000	GSP	6	0
5	P	2000	GSP	7	0
5	D	2000	GSP	6	0
5	B	2000	GSP	6	0
5	Z	2000	GSP	6	0
5	d	2000	GSP	11	0
5	h	2000	GSP	7	0
5	N	2000	GSP	6	0

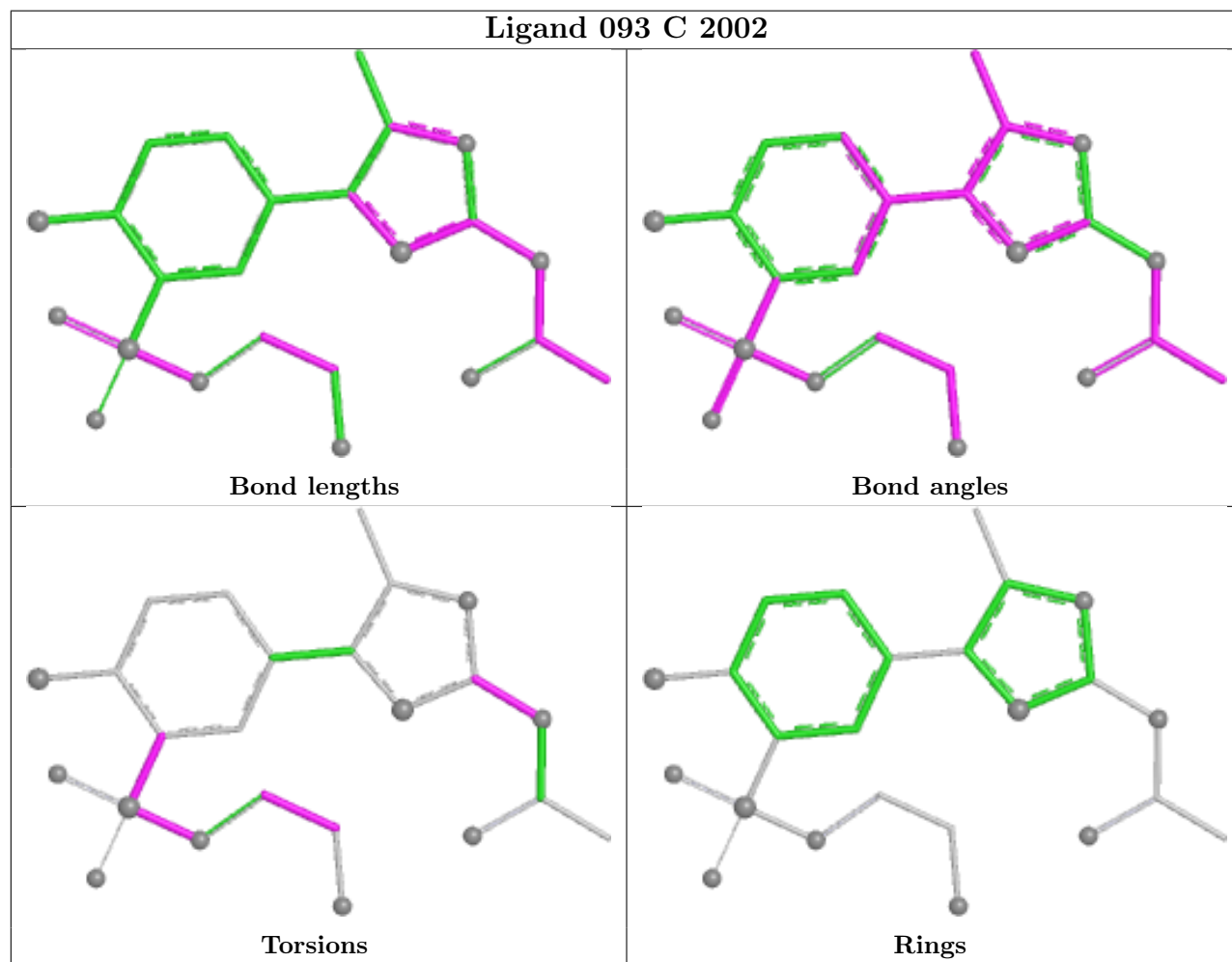
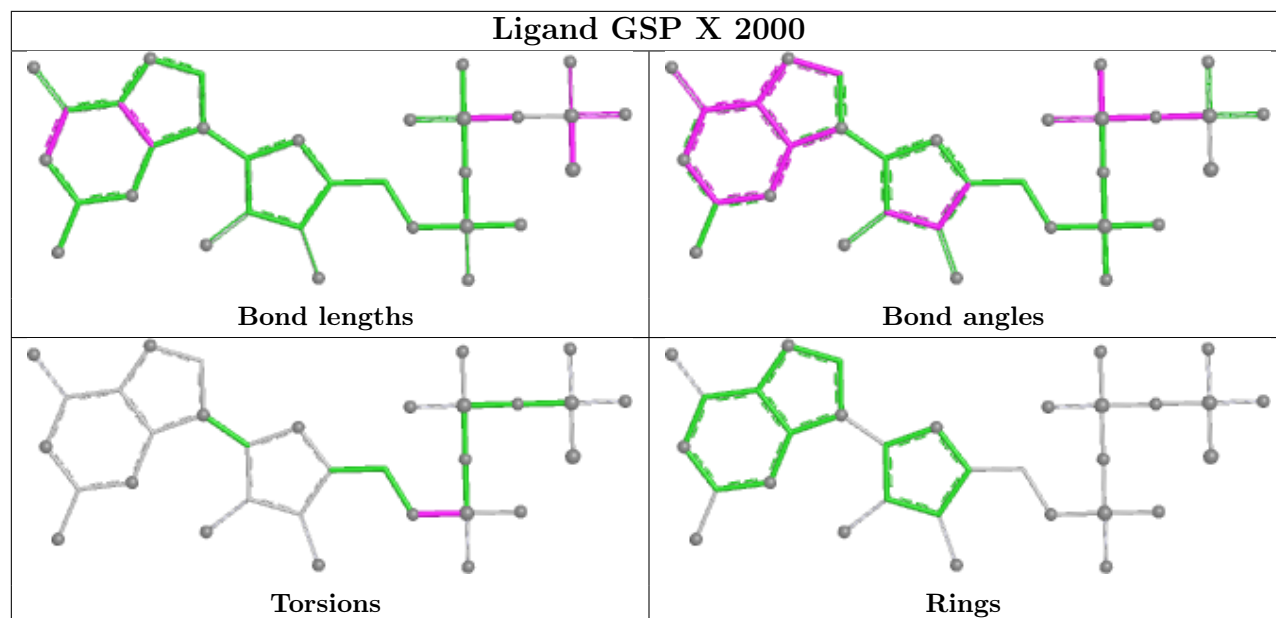
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

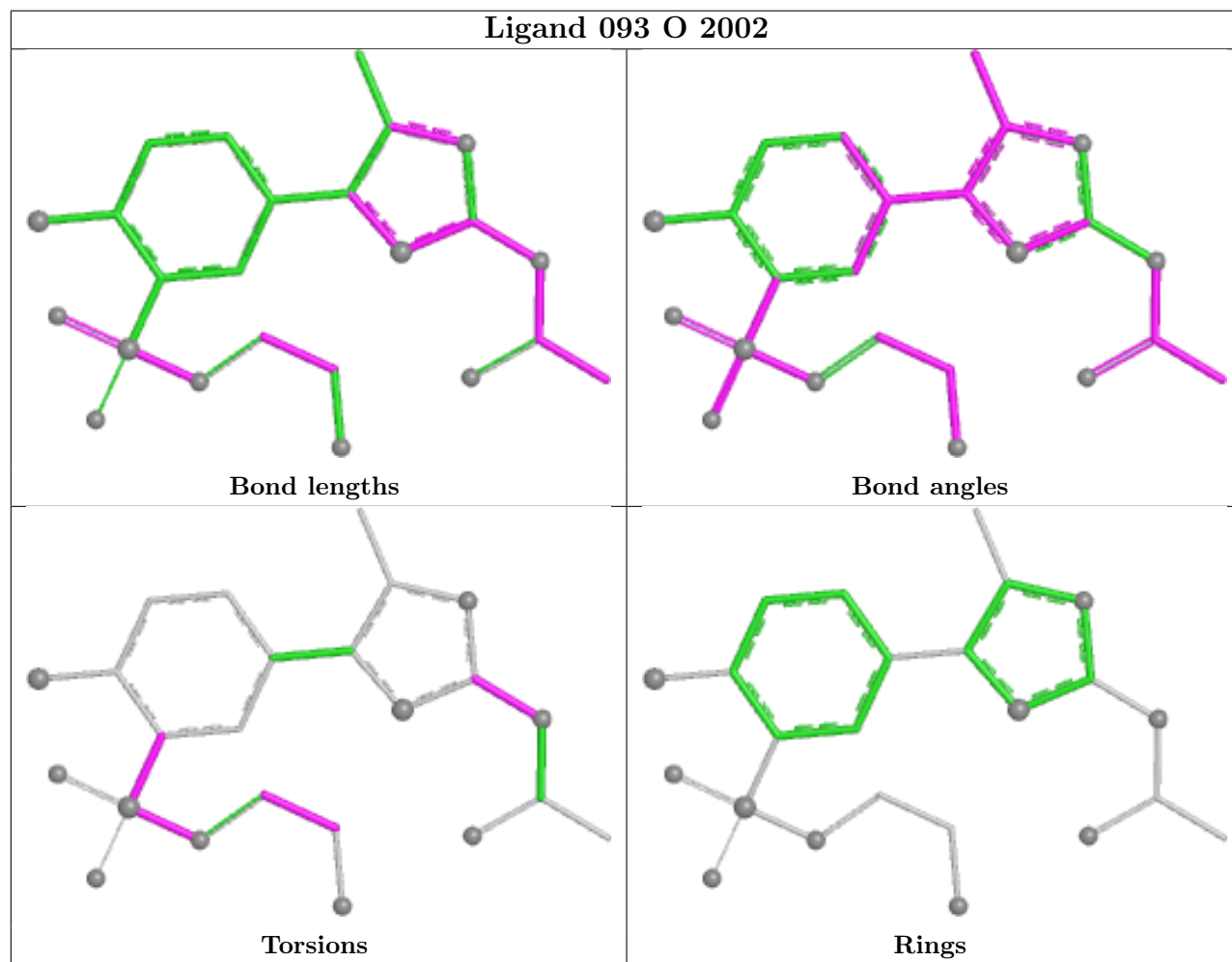
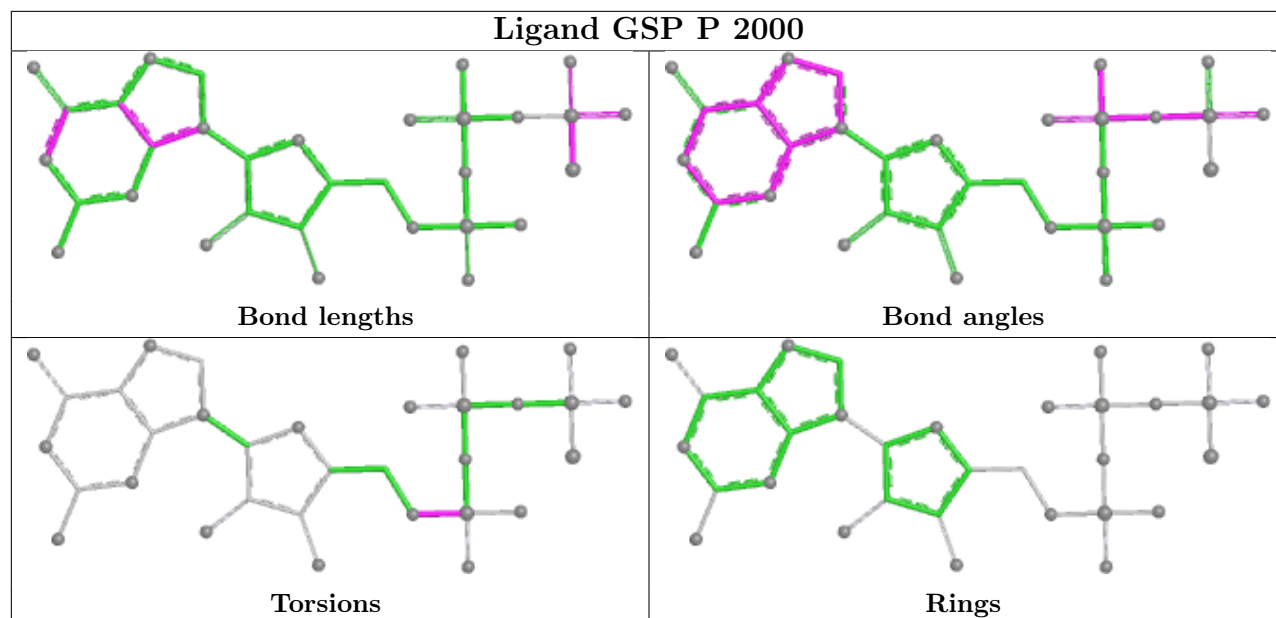


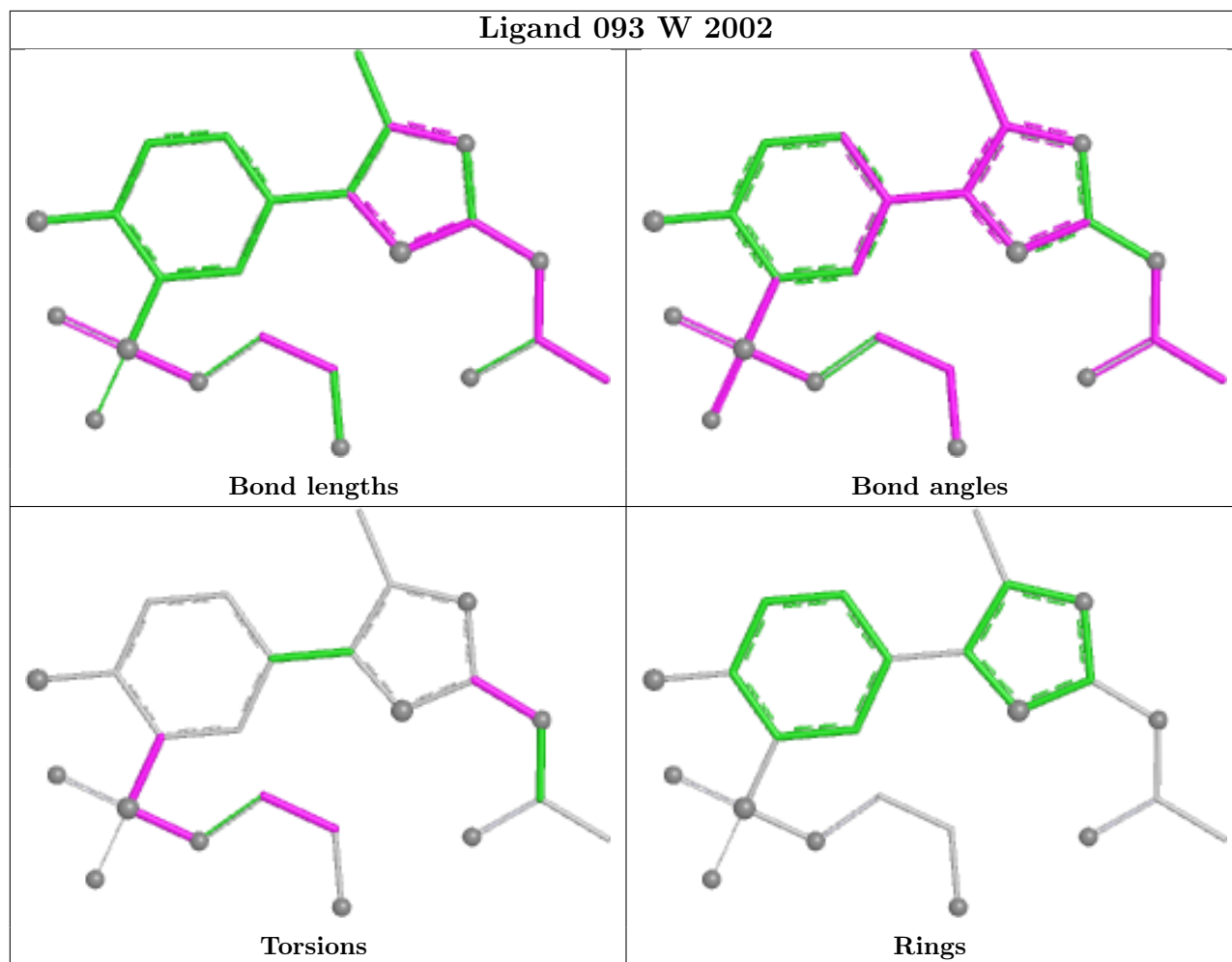


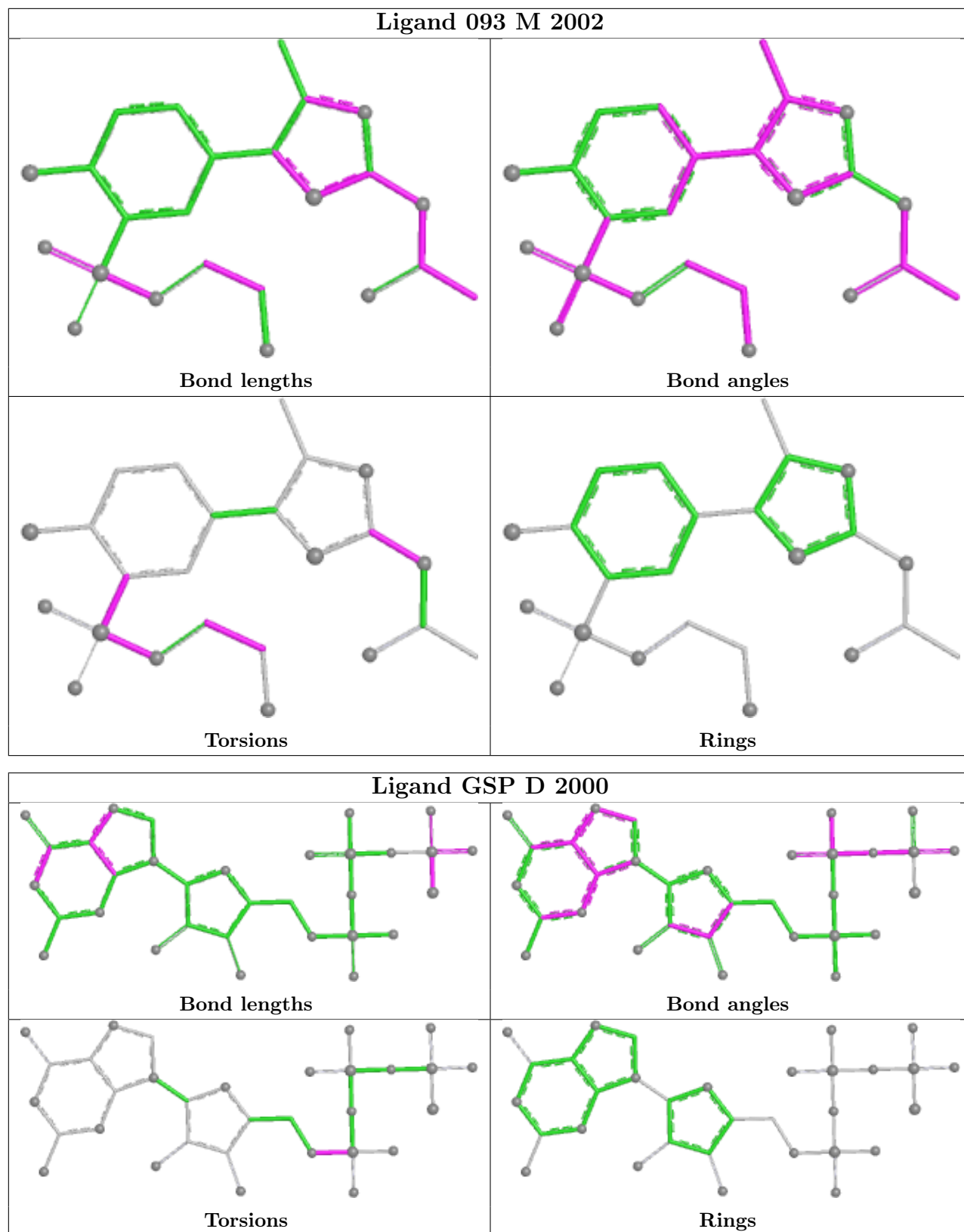


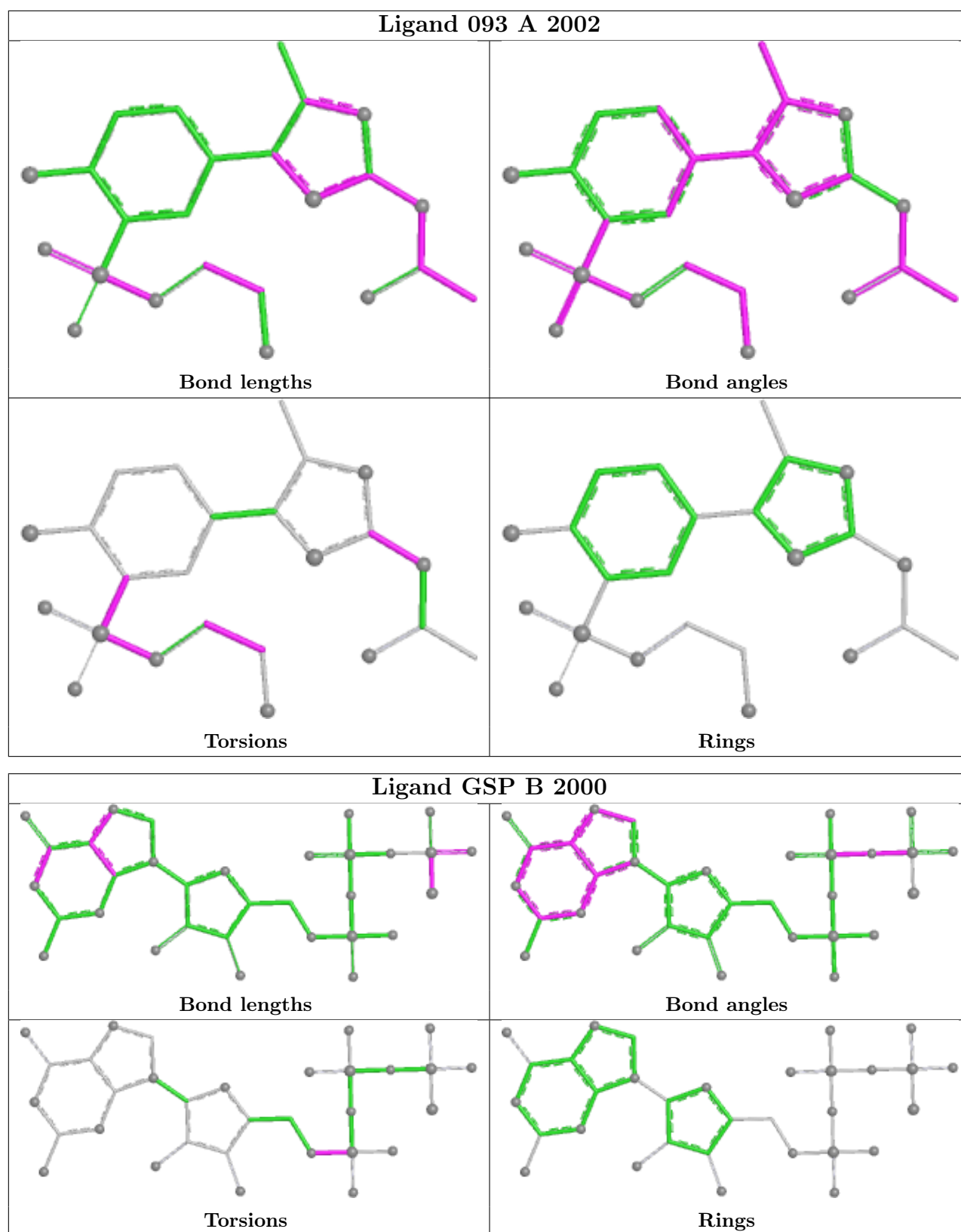


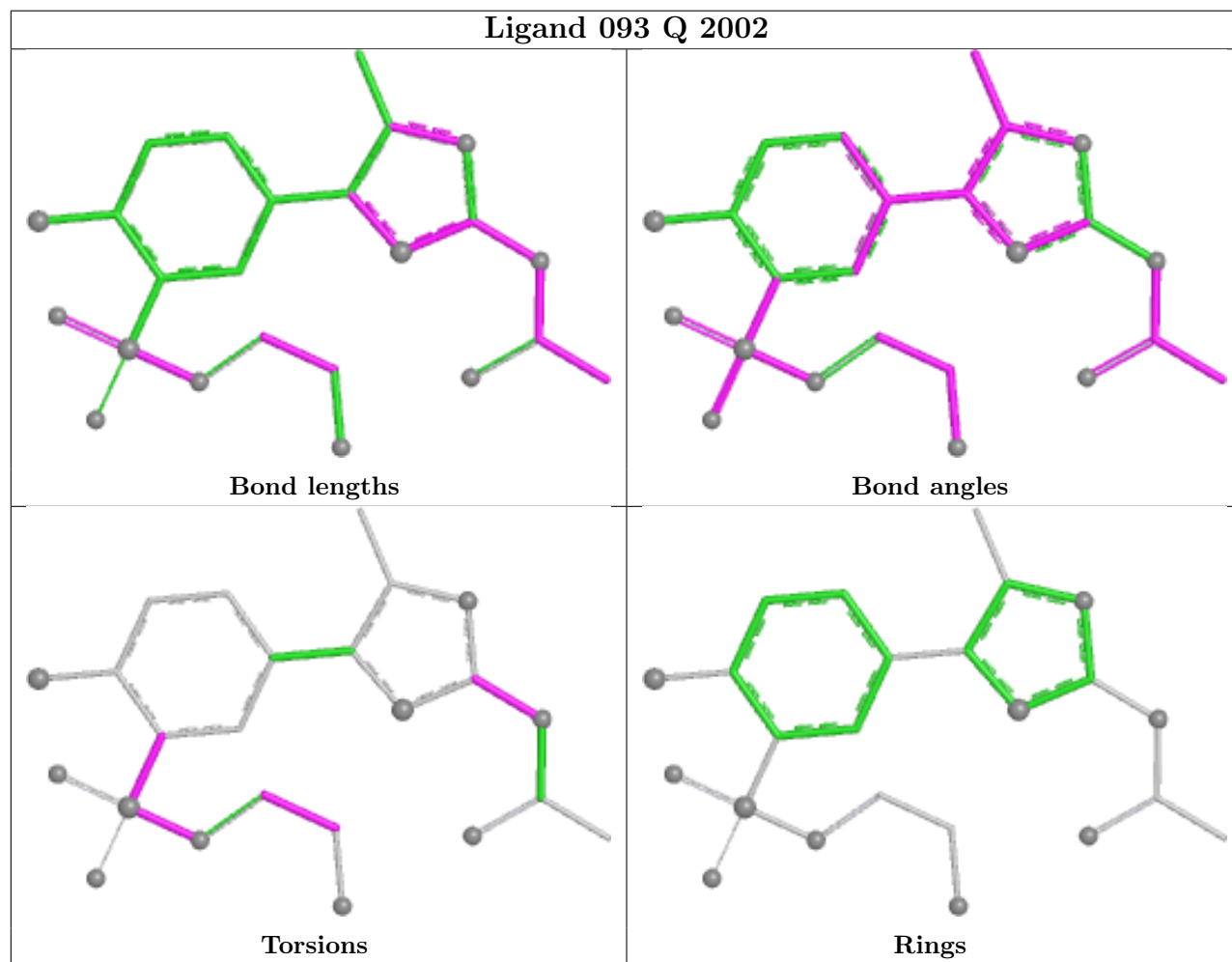
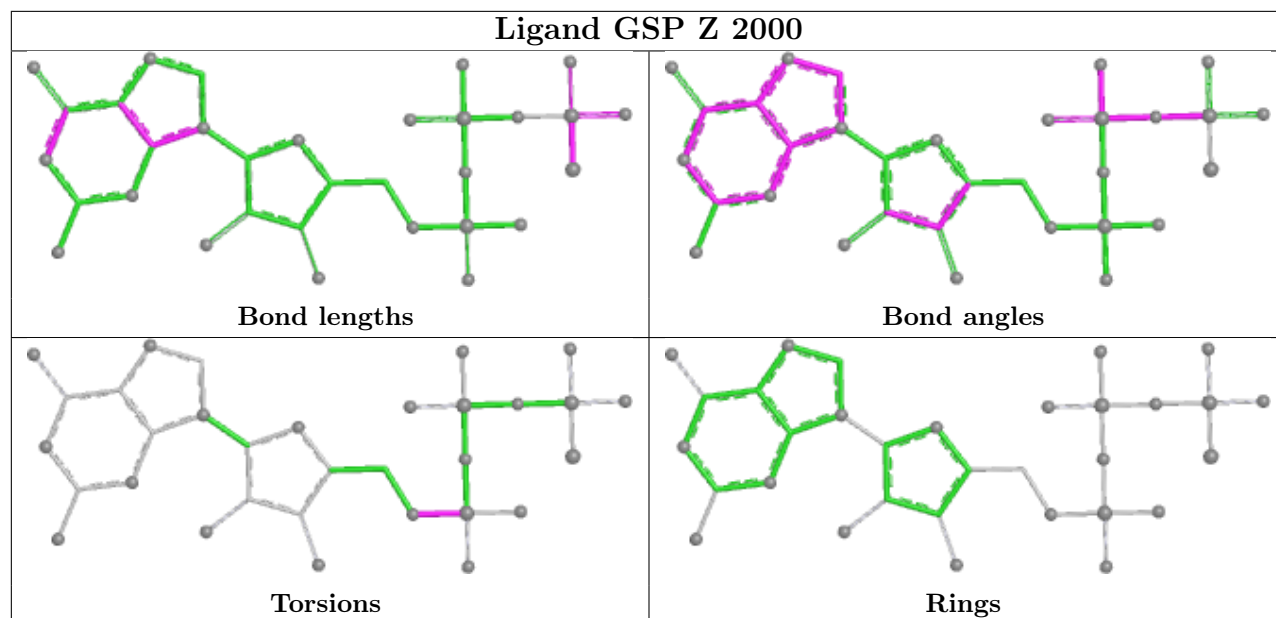


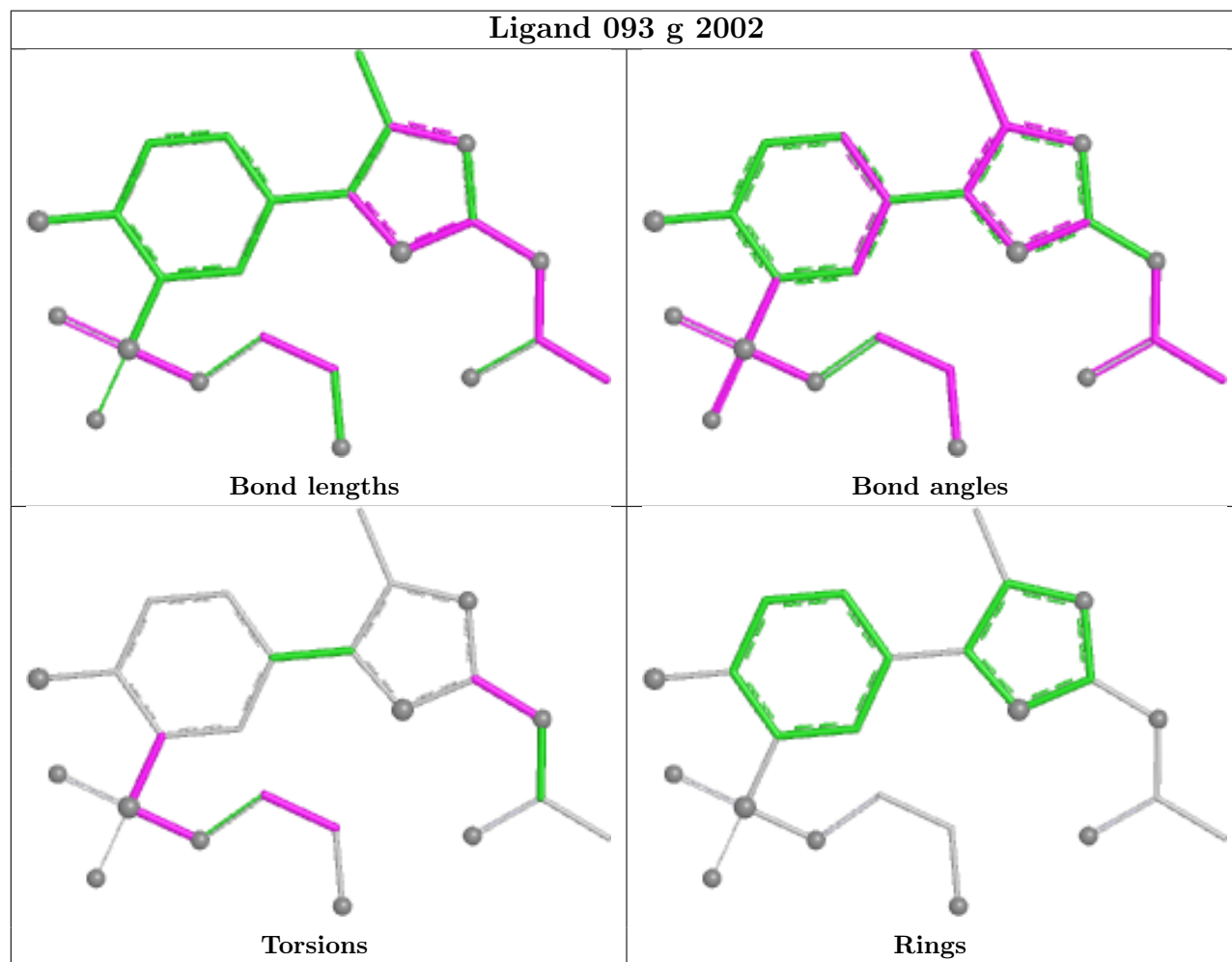
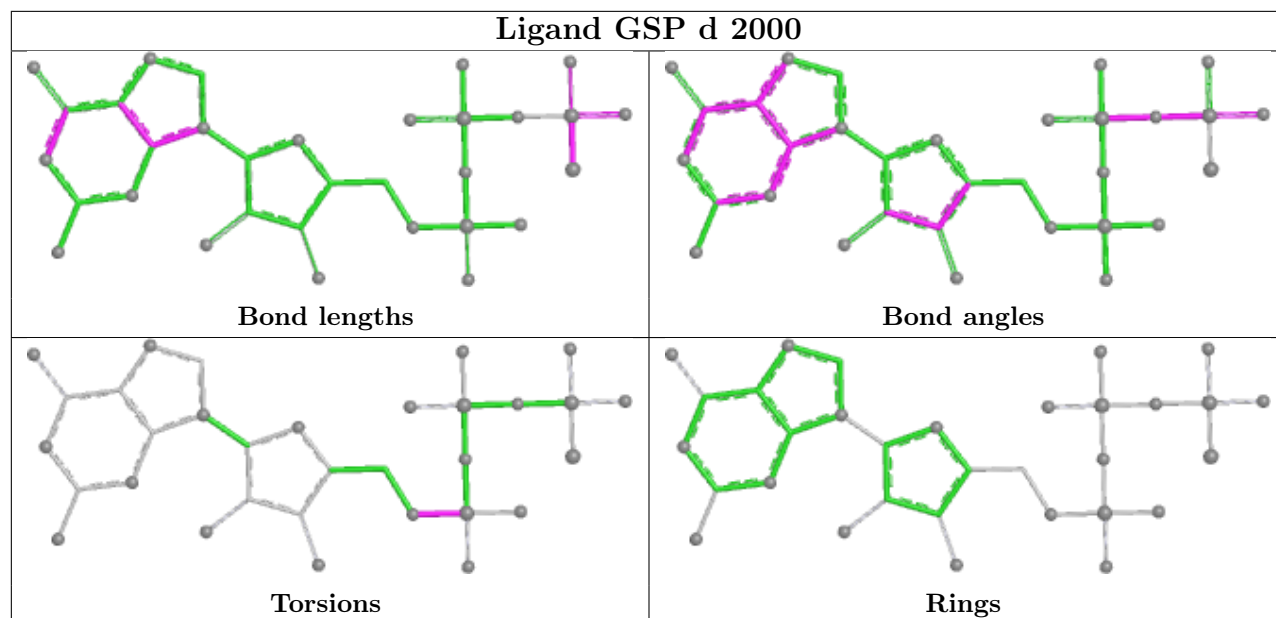


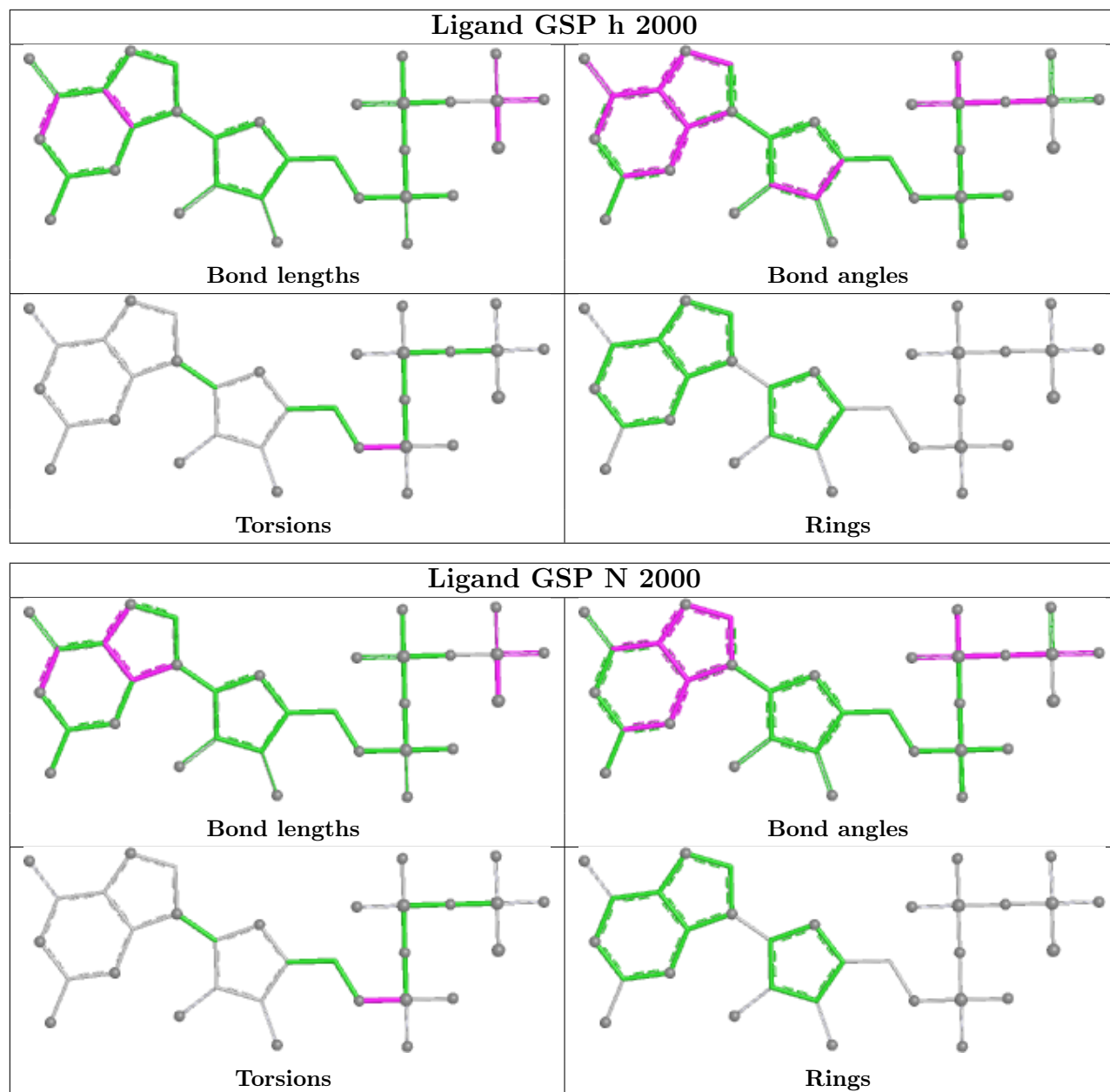


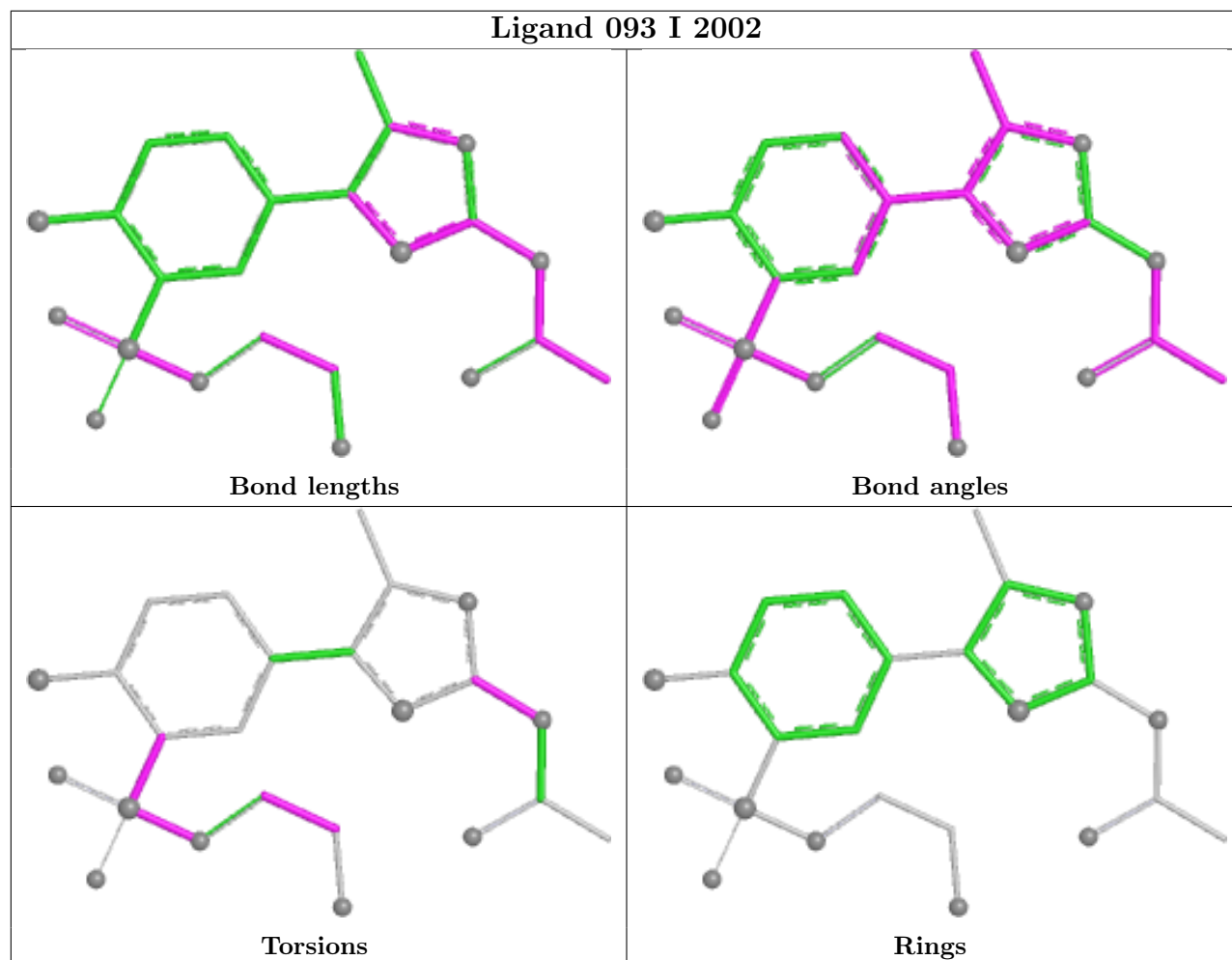


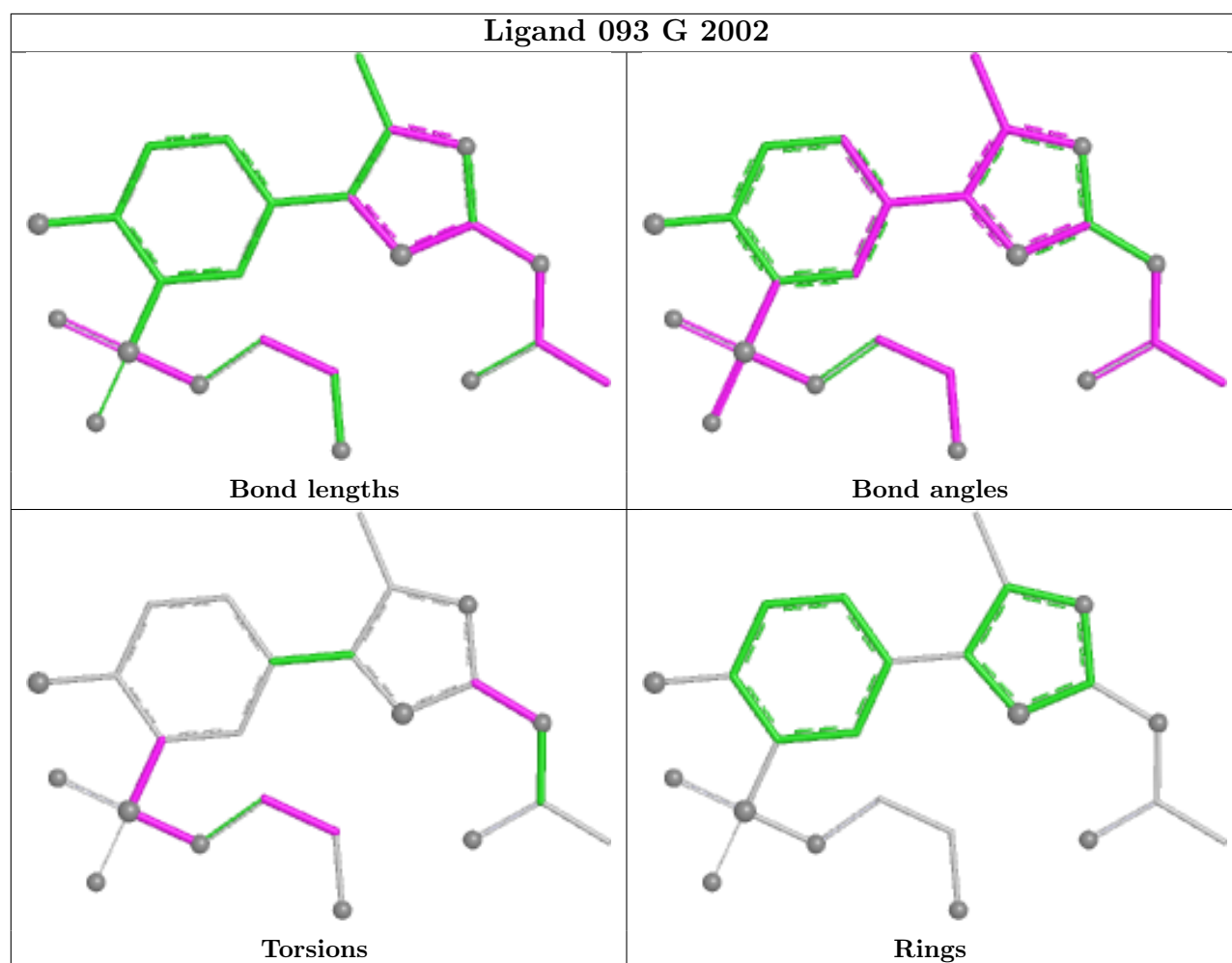












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/566 (83%)	-0.33	2 (0%) 88 79	95, 212, 331, 500	0
1	C	470/566 (83%)	-0.09	16 (3%) 48 43	126, 300, 456, 500	0
1	G	470/566 (83%)	-0.32	3 (0%) 85 75	98, 214, 342, 500	0
1	I	470/566 (83%)	-0.01	10 (2%) 63 54	124, 306, 474, 500	0
1	M	470/566 (83%)	-0.27	4 (0%) 81 70	95, 217, 341, 500	0
1	O	470/566 (83%)	-0.25	9 (1%) 66 56	102, 208, 335, 500	0
1	Q	470/566 (83%)	-0.19	4 (0%) 81 70	102, 247, 364, 498	0
1	S	470/566 (83%)	-0.14	9 (1%) 66 56	114, 251, 389, 500	0
1	W	470/566 (83%)	-0.13	12 (2%) 57 49	99, 253, 387, 500	0
1	Y	470/566 (83%)	-0.05	12 (2%) 57 49	115, 250, 364, 474	0
1	c	470/566 (83%)	-0.17	4 (0%) 81 70	119, 305, 478, 500	0
1	g	470/566 (83%)	-0.11	7 (1%) 72 60	126, 268, 416, 500	0
2	B	173/219 (78%)	-0.33	0 100 100	94, 201, 375, 493	0
2	D	173/219 (78%)	-0.10	3 (1%) 69 58	95, 220, 341, 488	0
2	H	173/219 (78%)	-0.21	2 (1%) 76 65	94, 207, 382, 499	0
2	J	173/219 (78%)	-0.28	2 (1%) 76 65	92, 198, 338, 500	0
2	N	173/219 (78%)	-0.19	1 (0%) 85 75	137, 282, 424, 496	0
2	P	173/219 (78%)	0.01	0 100 100	132, 277, 432, 496	0
2	R	173/219 (78%)	-0.02	6 (3%) 47 43	139, 269, 415, 496	0
2	T	173/219 (78%)	-0.11	2 (1%) 76 65	136, 266, 407, 493	0
2	X	173/219 (78%)	-0.02	3 (1%) 69 58	146, 282, 453, 500	0
2	Z	173/219 (78%)	0.12	5 (2%) 53 46	165, 262, 362, 494	0
2	d	173/219 (78%)	0.13	6 (3%) 47 43	146, 308, 447, 500	0
2	h	173/219 (78%)	0.06	7 (4%) 42 40	158, 294, 440, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	E	41/48 (85%)	-0.35	0 100 100	153, 251, 365, 489	0
3	F	32/48 (66%)	-0.10	1 (3%) 51 45	169, 285, 399, 466	0
3	K	41/48 (85%)	-0.27	0 100 100	131, 240, 410, 465	0
3	L	32/48 (66%)	-0.21	0 100 100	170, 263, 384, 436	0
3	U	41/48 (85%)	0.11	0 100 100	175, 284, 408, 494	0
3	V	32/48 (66%)	-0.47	0 100 100	170, 260, 403, 435	0
3	a	41/48 (85%)	-0.22	1 (2%) 59 51	195, 318, 423, 476	0
3	b	32/48 (66%)	-0.10	0 100 100	213, 309, 428, 479	0
3	e	41/48 (85%)	-0.16	0 100 100	175, 255, 384, 478	0
3	f	32/48 (66%)	-0.13	1 (3%) 51 45	194, 288, 337, 363	0
3	i	41/48 (85%)	-0.21	0 100 100	202, 325, 441, 500	0
3	j	32/48 (66%)	-0.02	0 100 100	194, 282, 404, 462	0
All	All	8154/9996 (81%)	-0.15	132 (1%) 70 59	92, 255, 416, 500	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	775	GLU	6.0
1	M	707	ASP	4.8
2	X	84	ALA	4.8
1	Q	624	GLY	4.4
1	C	721	GLY	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

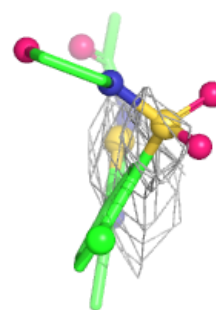
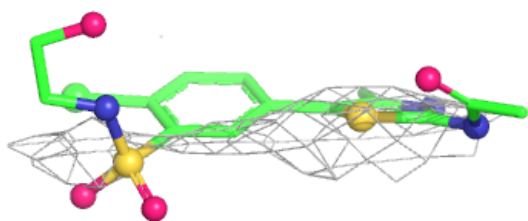
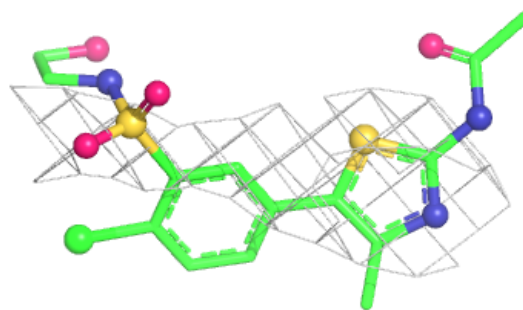
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	093	A	2002	24/24	-	-	60,76,105,130	24
4	093	C	2002	24/24	-	-	60,76,105,130	24
4	093	G	2002	24/24	-	-	60,76,105,130	24
4	093	I	2002	24/24	-	-	60,76,105,130	24
4	093	M	2002	24/24	-	-	60,76,105,130	24
4	093	O	2002	24/24	-	-	60,76,105,130	24
4	093	Q	2002	24/24	-	-	60,76,105,130	24
4	093	S	2002	24/24	-	-	60,76,105,130	24
4	093	W	2002	24/24	-	-	60,76,105,130	24
4	093	Y	2002	24/24	-	-	60,76,105,130	24
4	093	c	2002	24/24	-	-	60,76,105,130	24
4	093	g	2002	24/24	-	-	60,76,105,130	24
5	GSP	J	2000	32/32	0.95	0.09	94,165,285,323	0
6	MG	X	2001	1/1	0.95	0.06	255,255,255,255	0
5	GSP	X	2000	32/32	0.97	0.07	134,226,322,330	0
5	GSP	R	2000	32/32	0.97	0.07	108,197,262,274	0
5	GSP	P	2000	32/32	0.98	0.07	111,168,247,275	0
5	GSP	D	2000	32/32	0.98	0.07	110,193,250,272	0
5	GSP	T	2000	32/32	0.98	0.07	123,205,238,264	0
5	GSP	H	2000	32/32	0.98	0.05	141,183,247,282	0
5	GSP	d	2000	32/32	0.98	0.07	174,212,349,391	0
5	GSP	h	2000	32/32	0.98	0.07	123,249,350,363	0
6	MG	H	2001	1/1	0.98	0.04	139,139,139,139	0
6	MG	N	2001	1/1	0.98	0.07	240,240,240,240	0
5	GSP	B	2000	32/32	0.98	0.05	141,197,232,249	0
6	MG	h	2001	1/1	0.98	0.04	190,190,190,190	0
6	MG	J	2001	1/1	0.99	0.06	142,142,142,142	0
5	GSP	Z	2000	32/32	0.99	0.07	176,212,274,298	0
6	MG	R	2001	1/1	0.99	0.03	106,106,106,106	0
6	MG	T	2001	1/1	0.99	0.03	127,127,127,127	0
6	MG	B	2001	1/1	0.99	0.03	159,159,159,159	0
6	MG	Z	2001	1/1	0.99	0.05	178,178,178,178	0
6	MG	d	2001	1/1	0.99	0.05	167,167,167,167	0
5	GSP	N	2000	32/32	0.99	0.05	97,151,255,301	0
6	MG	D	2001	1/1	1.00	0.04	64,64,64,64	0
6	MG	P	2001	1/1	1.00	0.10	244,244,244,244	0

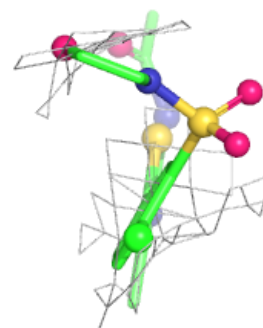
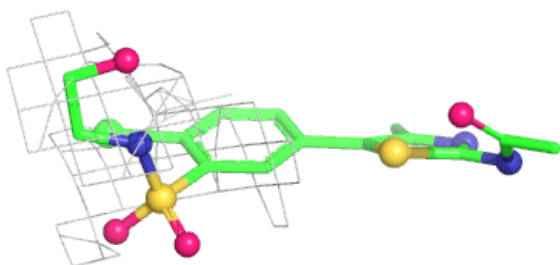
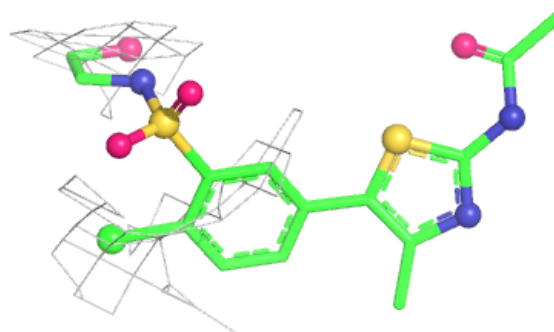
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 093 A 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

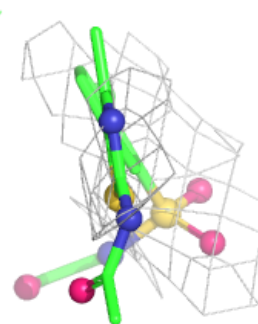
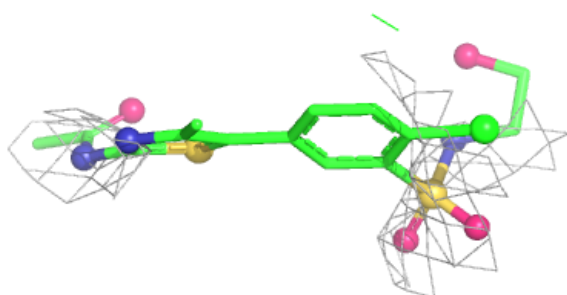
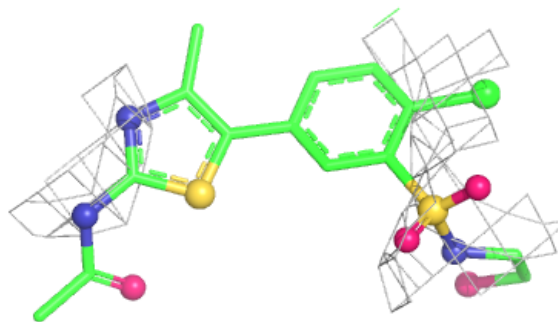
**Electron density around 093 C 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

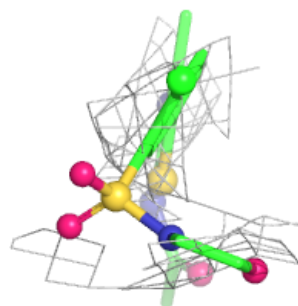
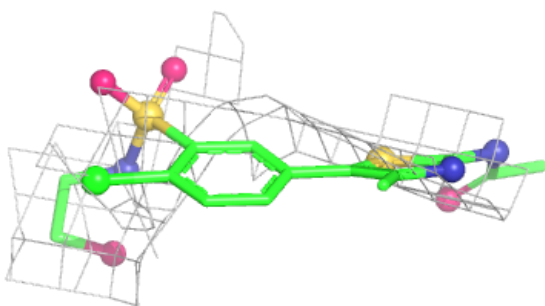
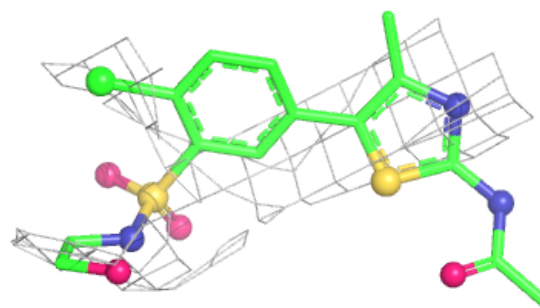


Electron density around 093 G 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

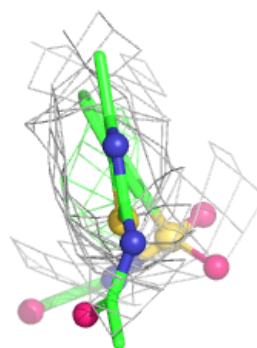
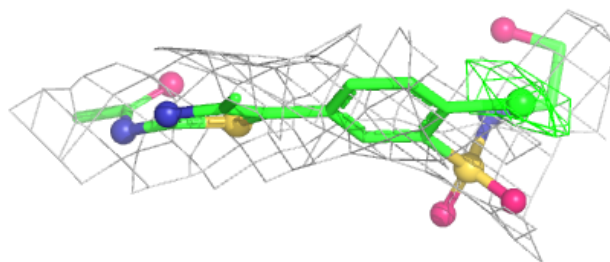
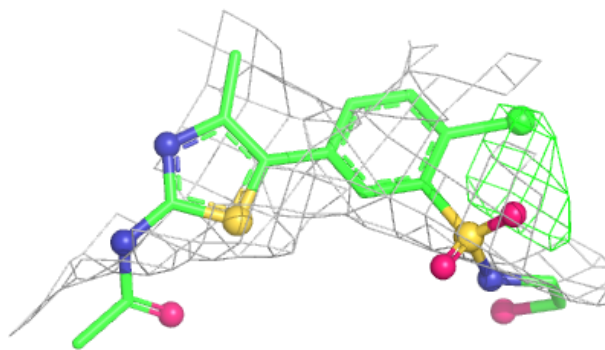
**Electron density around 093 I 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

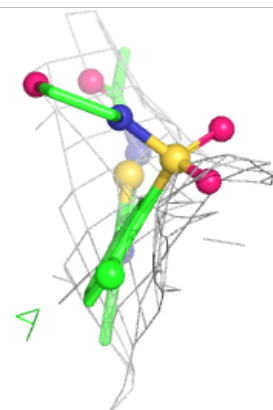
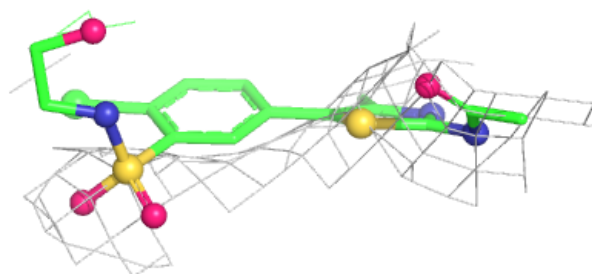
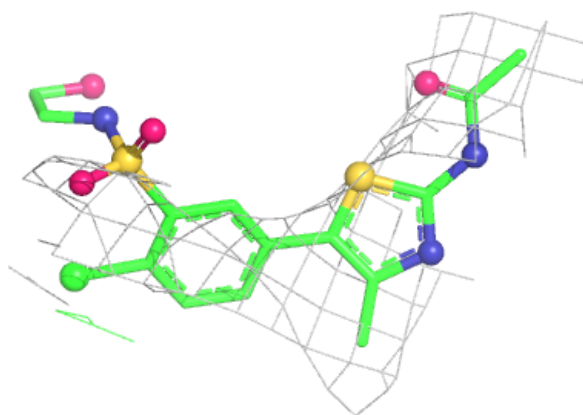


Electron density around 093 M 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

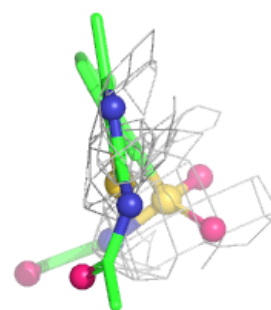
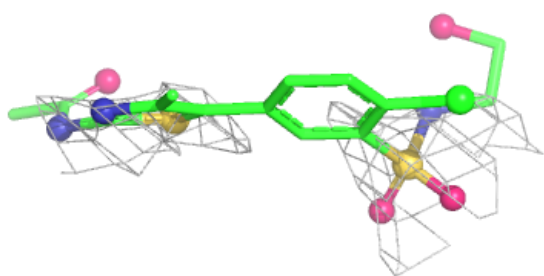
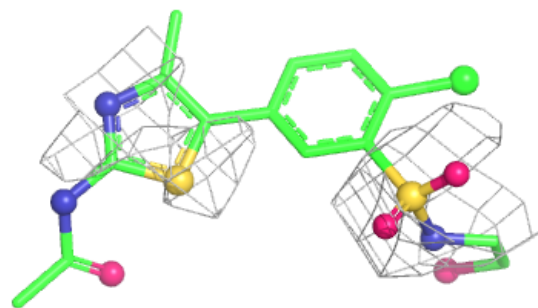
**Electron density around 093 O 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

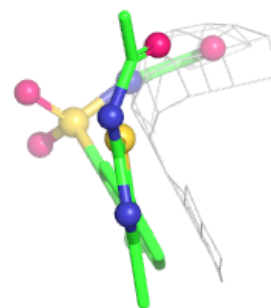
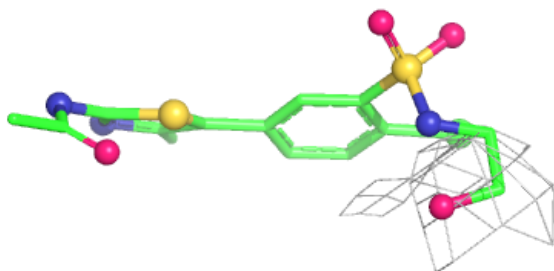
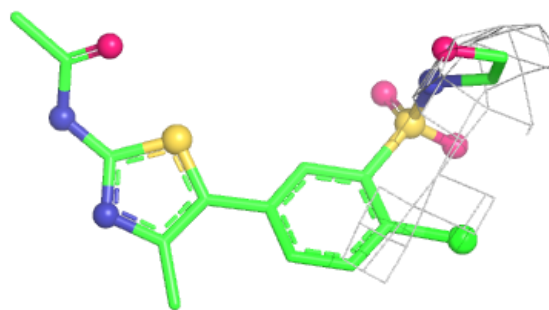


Electron density around 093 Q 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

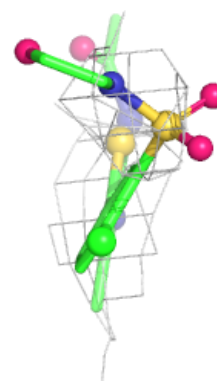
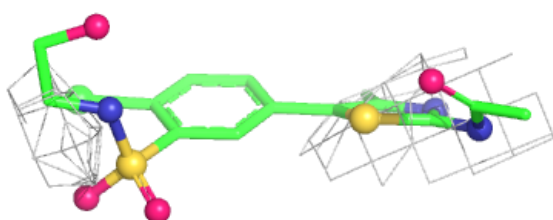
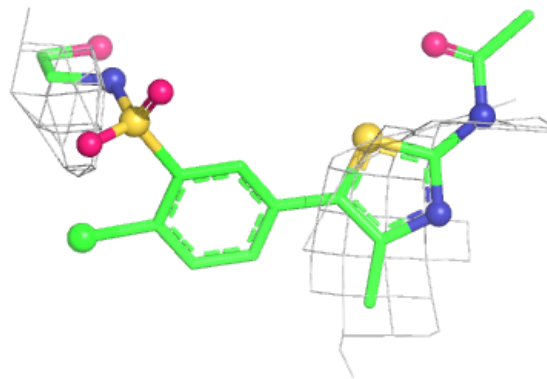
**Electron density around 093 S 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

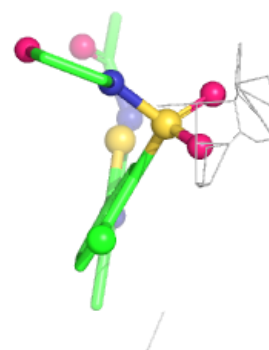
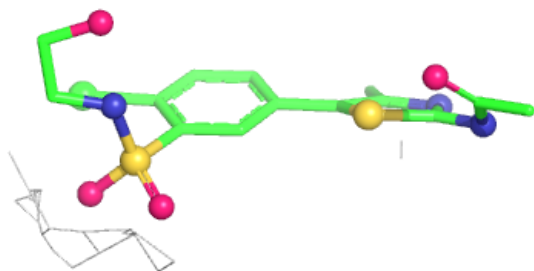
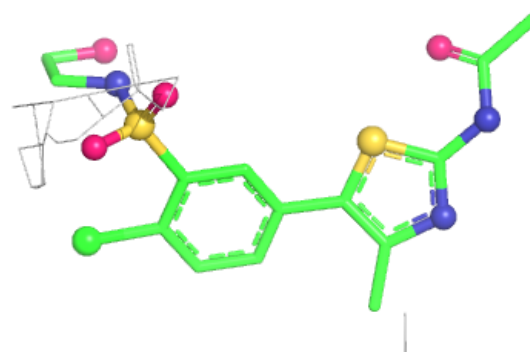


Electron density around 093 W 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

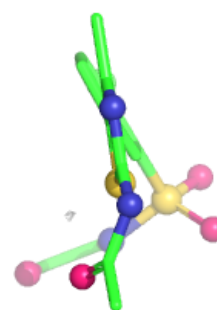
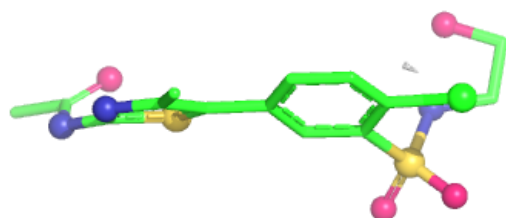
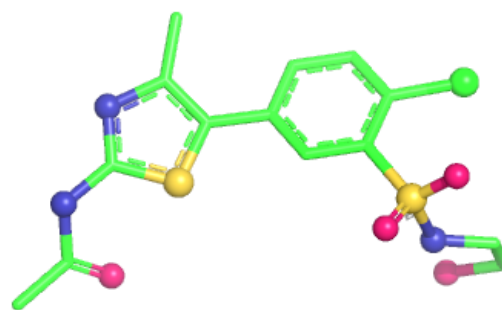
**Electron density around 093 Y 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

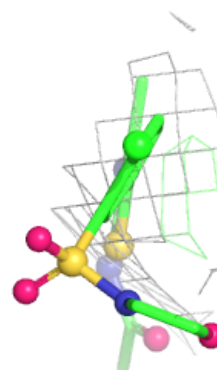
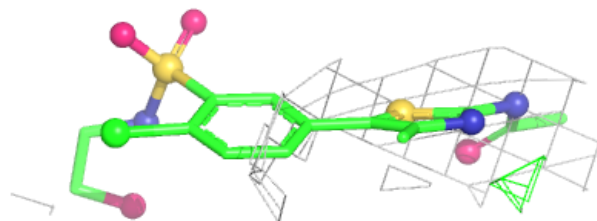
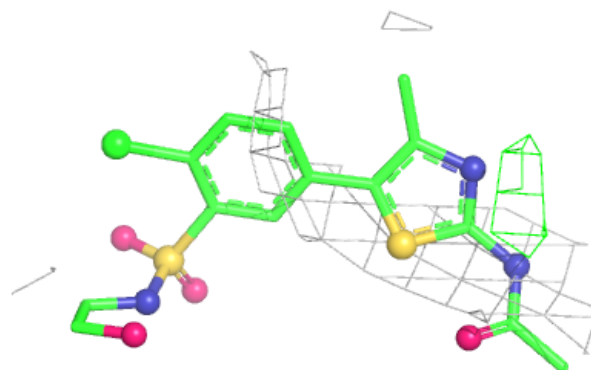


Electron density around 093 c 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

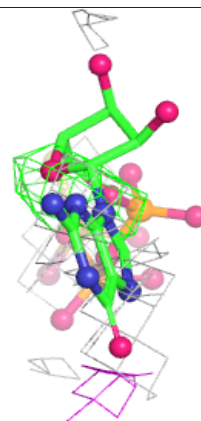
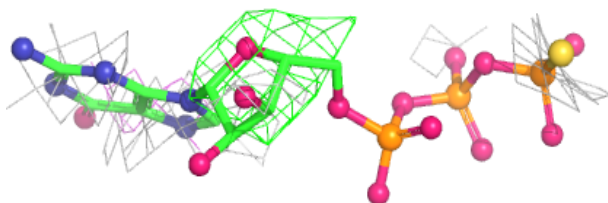
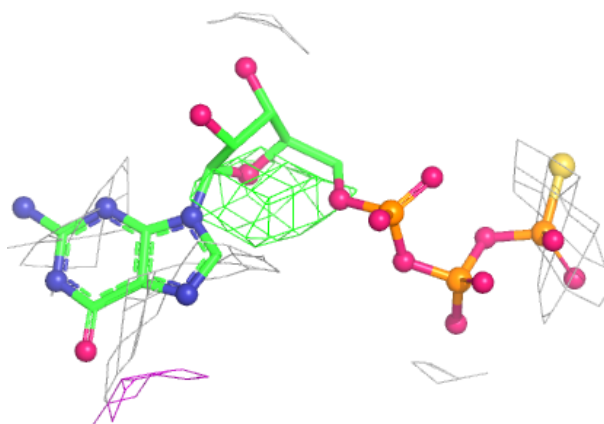
**Electron density around 093 g 2002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

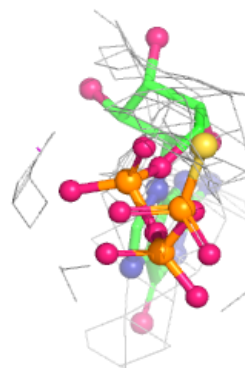
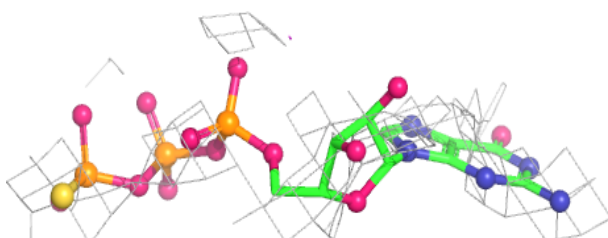
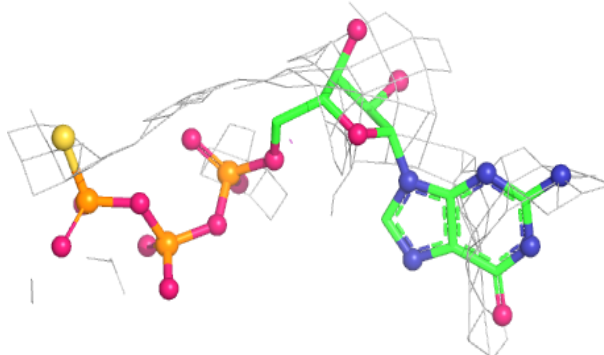


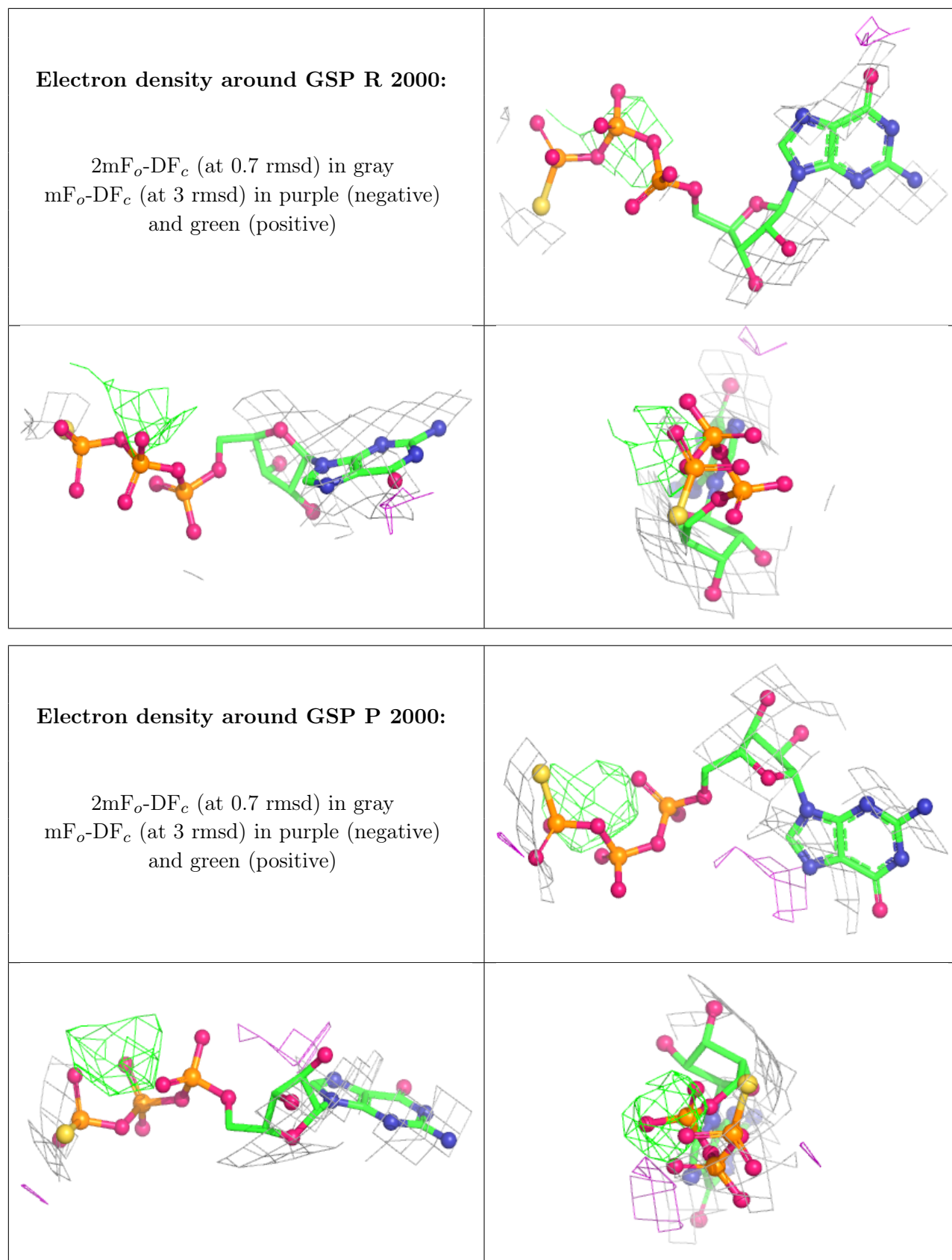
Electron density around GSP J 2000:

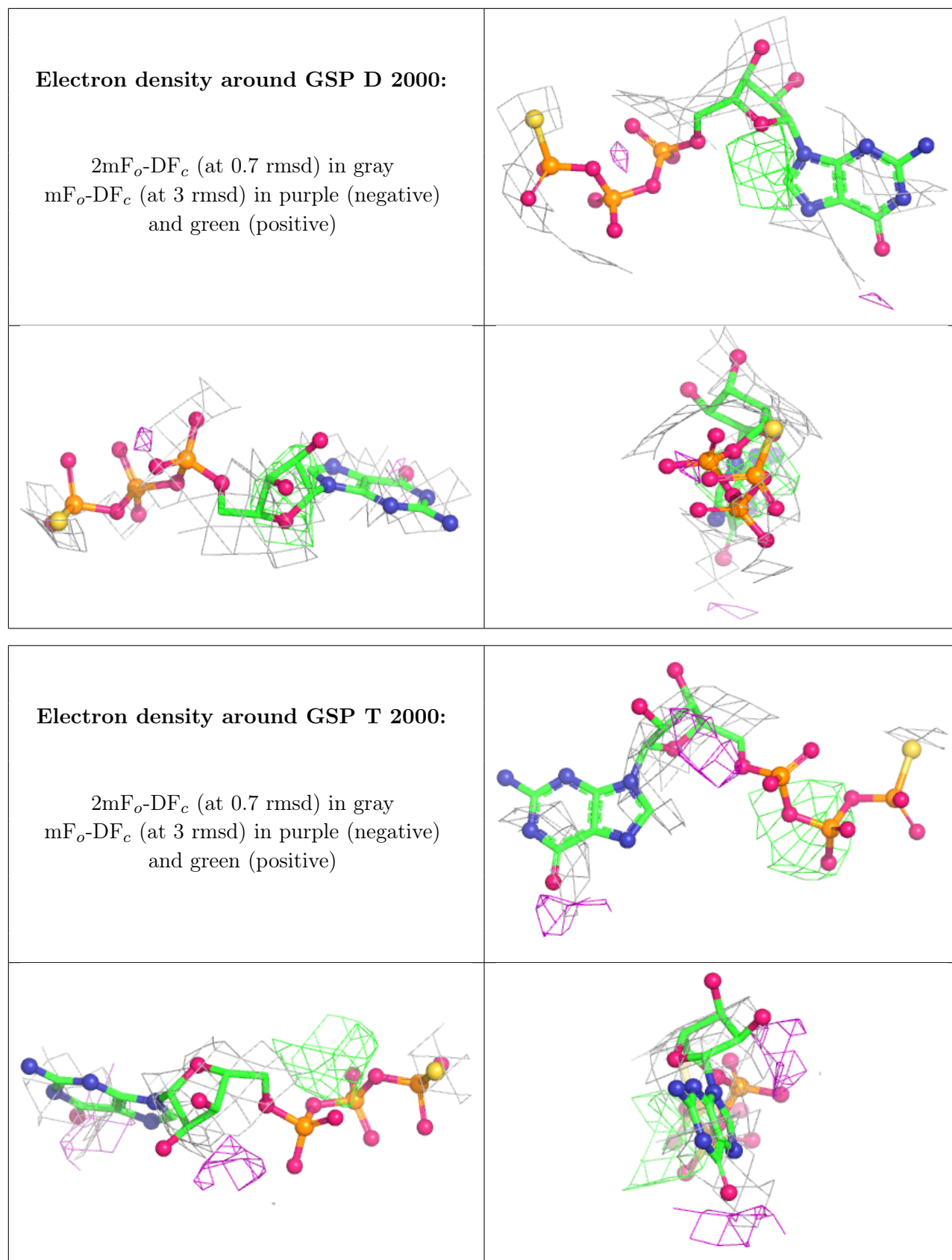
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GSP X 2000:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

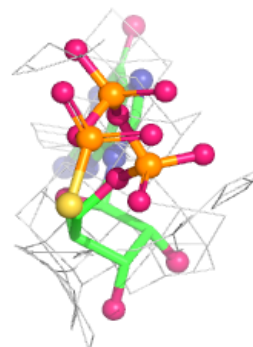
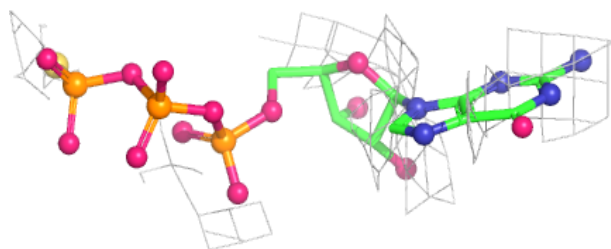
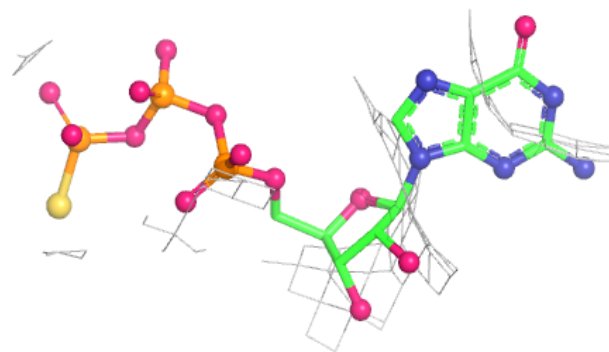




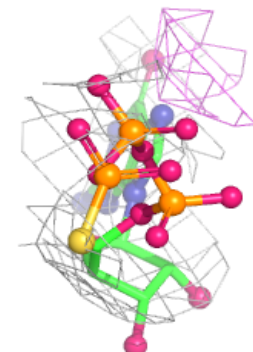
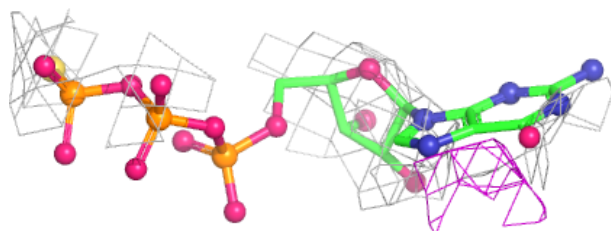
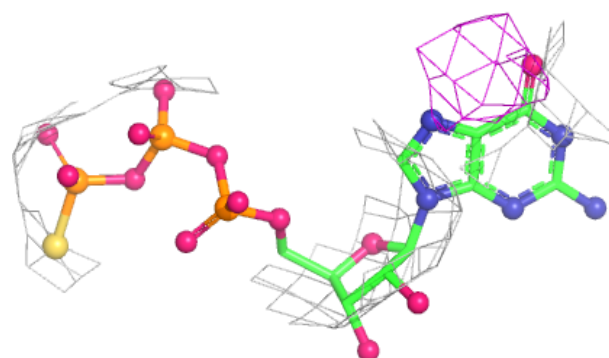


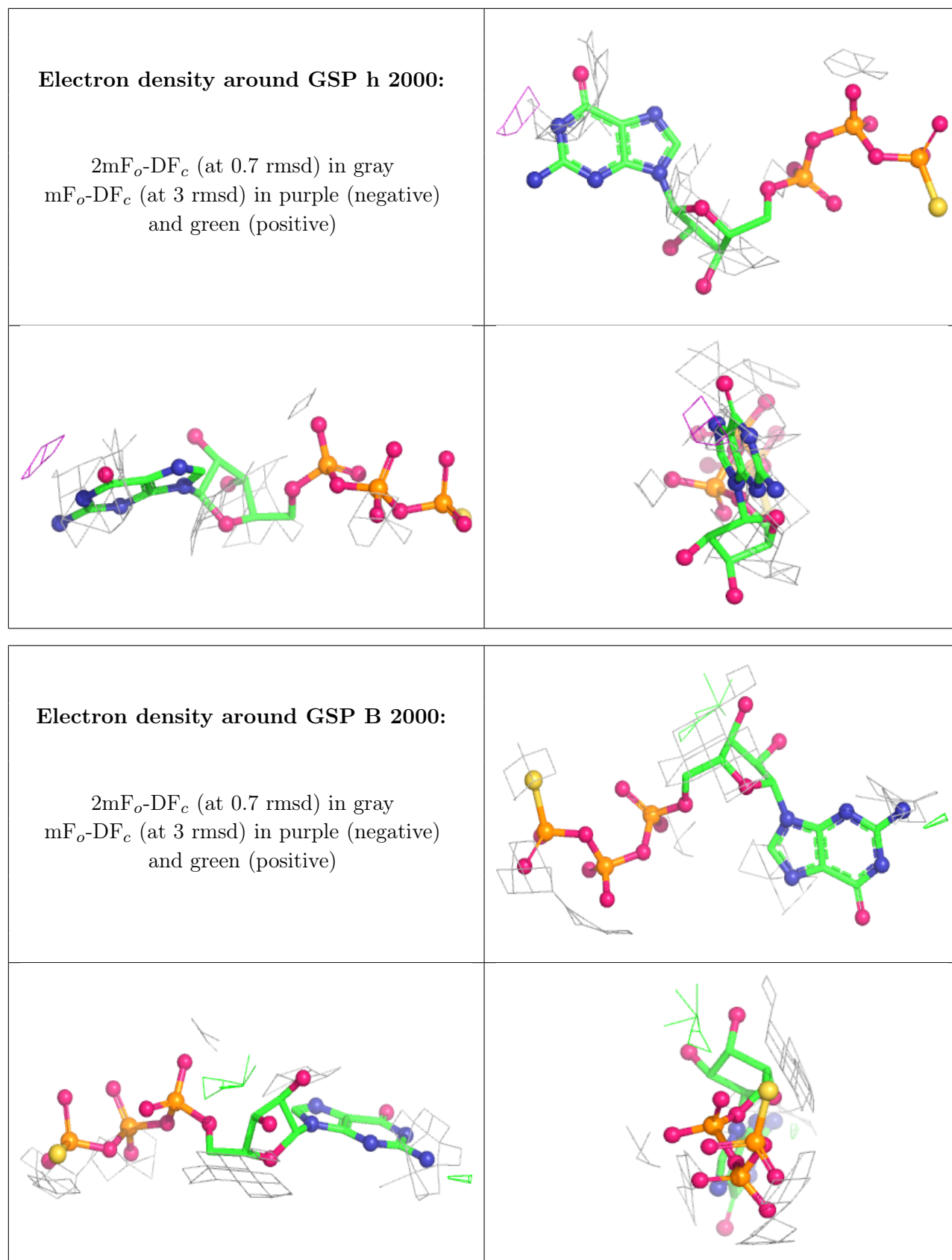
Electron density around GSP H 2000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GSP d 2000:**

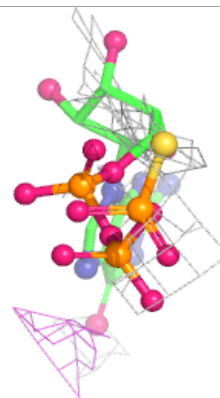
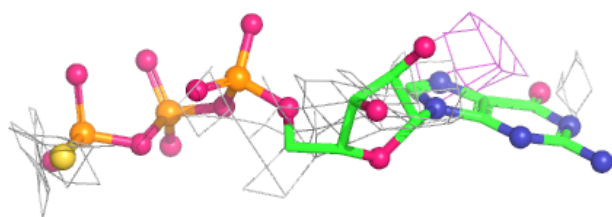
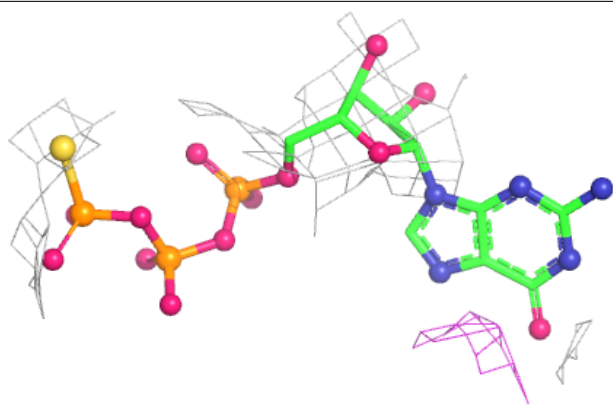
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



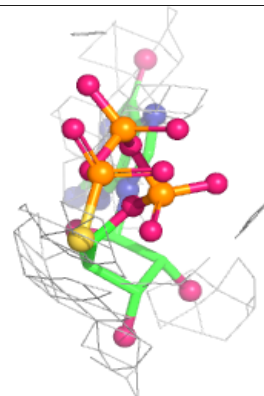
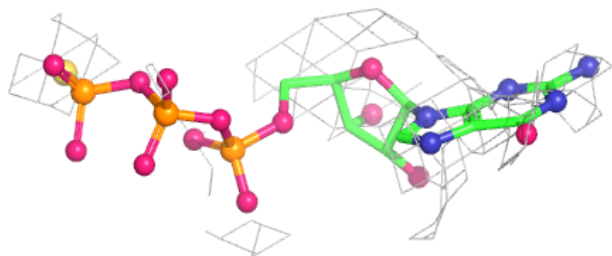
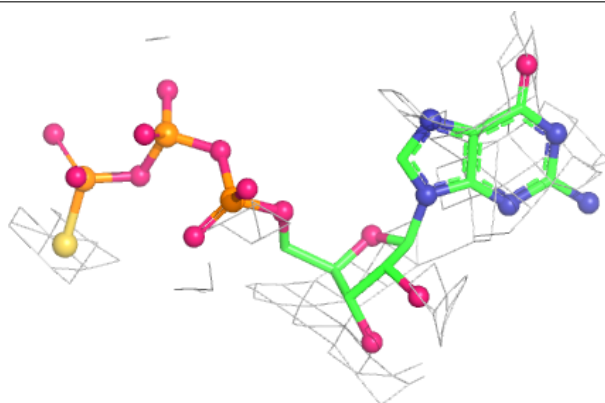


Electron density around GSP Z 2000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GSP N 2000:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.